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DICTIONARY FILE UPDATES:  25 MAR 2008  HIGHEST RN 1010115-69-1

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FILE COVERS 1907 - 26 Mar 2008  VOL 148 ISS 13
FILE LAST UPDATED: 25 Mar 2008  (20080325/ED)

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  substance identification.
'OBI' IS DEFAULT SEARCH FIELD FOR 'ZCAPLUS' FILE

=> d stat que L38
L35       17804 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  TANAKA S?/AU
L36        5183 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  FUKUDA K?/AU
L37         998 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  ASADA T?/AU
L38           1 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  L35 AND L36 AND L37
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=> d stat que L43
L32       36798 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  ?PERFUM?/BI
L35       17804 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  TANAKA S?/AU
L36        5183 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  FUKUDA K?/AU
L37         998 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  ASADA T?/AU
L39          41 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  L35 AND (L36 OR L37)
L43          11 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  L39 AND L32


=> file wpix
FILE 'WPIX' ENTERED AT 16:56:54 ON 26 MAR 2008
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FILE LAST UPDATED:                          24 MAR 2008   <20080324/UP>
MOST RECENT THOMSON SCIENTIFIC UPDATE:     200820      <200820/DW>
DERWENT WORLD PATENTS INDEX SUBSCRIBER FILE, COVERS 1963 TO DATE

>>> IPC Reform backfile reclassification has been loaded to the end of
    November 2007. No update date (UP) has been created for the
    reclassified documents, but they can be identified by
    20060101/UPIC and 20061231/UPIC, 20070601/UPIC, 20071001/UPIC and
    20071130/UPIC. <<<

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FOR DETAILS OF THE PATENTS COVERED IN CURRENT UPDATES, SEE
http://scientific.thomson.com/support/patents/coverage/latestupdates/

EXPLORE DERWENT WORLD PATENTS INDEX IN STN ANAVIST, VERSION 2.0:
http://www.stn-international.com/archive/presentations/DWPIAnaVist2_0710.pdf

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>>> Updated PDF files in the following links:
    http://www.stn-international.de/stndatabases/details/ico_0801.zip
    http://www.stn-international.de/stndatabases/details/epc_0801.zip
    Supplement of all changed ECLA items:
    http://www.stn-international.de/stndatabases/details/ecla_0802s.zip <<<
'BIX' IS DEFAULT SEARCH FIELD FOR 'WPIX' FILE

=> s L43
         17396 TANAKA S?/AU
          5776 FUKUDA K?/AU
          1486 ASADA T?/AU
         30920 ?PERFUM?/BI
L49         10 L39 AND L32


=> dup rem L38 L39 L49
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PROCESSING COMPLETED FOR L38
PROCESSING COMPLETED FOR L39
PROCESSING COMPLETED FOR L49
L50          41 DUP REM L38 L39 L49 (11 DUPLICATES REMOVED)
                ANSWERS '1-41' FROM FILE ZCAPLUS

=> dup rem L38 L43 L49
PROCESSING COMPLETED FOR L38
PROCESSING COMPLETED FOR L43
PROCESSING COMPLETED FOR L49
L51          11 DUP REM L38 L43 L49 (11 DUPLICATES REMOVED)
                ANSWERS '1-11' FROM FILE ZCAPLUS

=> d ibib abs hitind hitstr L51 1-11

L51  ANSWER 1 OF 11  ZCAPLUS  COPYRIGHT 2008 ACS on STN DUPLICATE 1
ACCESSION NUMBER:         2007:618990  ZCAPLUS  Full-text
DOCUMENT NUMBER:          147:30745
TITLE:                    Process for preparation of α,β-unsaturated
                          aldehydes via intramolecular condensation of aldehydes
                          in the presence of amines and proton acids.
INVENTOR(S):              Ishida, Kosaku; Tanaka, Shigeyoshi; Asada, Takahiro
PATENT ASSIGNEE(S):       Kao Corporation, Japan
SOURCE:                   PCT Int. Appl., 28pp.
                          CODEN: PIXXD2
DOCUMENT TYPE:            Patent
LANGUAGE:                 English
FAMILY ACC. NUM. COUNT:   1
PATENT INFORMATION:

     PATENT NO.            KIND   DATE        APPLICATION NO.          DATE
     ---------------       ----   --------    --------------------     --------
     WO 2007063703          A1    20070607    WO 2006-JP322699         20061108
         W:  AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH,
             CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,
             GE, GH, GM, GT, HN, HR, HU, ID, IL, IN, IS, KE, KG, KM, KN, KP,
             KR, KZ, LA, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN,
             MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS,
             RU, SC, SD, SE, SG, SK, SL, SM, SV, SY, TJ, TM, TN, TR, TT, TZ,
             UA, UG, US, UZ, VC, VN, ZA, ZM, ZW
         RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE,
             IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ,
             CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH,
             GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
             KG, KZ, MD, RU, TJ, TM
     JP 2007153764          A     20070621    JP 2005-348121           20051201
PRIORITY APPLN. INFO.:                       JP 2005-348121      A    20051201
OTHER SOURCE(S):          CASREACT 147:30745
AB   A process for preparation of α,β-unsatd. aldehydes comprises subjecting
     aldehydes to an intermol. condensation reaction in the presence of an amine
     and a protonic acid having 4-20 C atoms or a salt thereof. Thus, a mixture of
     campholenic aldehyde, piperidine, and stearic acid at 100° was treated with
     propionaldehyde over 6 h to give 95% 2-methyl-4-(2,2,3-trimethylcyclopent-3-
     en-1-yl)but-2-en-1-al of 60.6% purity.  The latter was purified by
     distillation and reduced with LiAlH4 in Et2O to give 85% 2-methyl-4-(2,2,3-
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trimethylcyclopent-3-en-1-yl)but-2-en-1-ol. This had a sandalwood scent and was excellent as a perfume material.
CC 24-4 (Alicyclic Compounds)
Section cross-reference(s): 30, 62
ST aldehyde unsatd prepn; alc unsatd perfume; aldol condensation amine protonic base
IT Perfumes
(unsatd. alcs.)
REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L51 ANSWER 2 OF 11 ZCAPLUS COPYRIGHT 2008 ACS on STN DUPLICATE 2
ACCESSION NUMBER: 2004:292019 ZCAPLUS Full-text
DOCUMENT NUMBER: 140:321236
TITLE: Preparation of valerolactone compounds and perfume composition
INVENTOR(S): Tanaka, Sakuya; Fukuda, Kazuyuki; Azada, Takahiro
PATENT ASSIGNEE(S): Kao Corporation, Japan
SOURCE: PCT Int. Appl., 65 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004029033	A1	20040408	WO 2003-JP12341	20030926
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
JP 2004161746	A	20040610	JP 2003-323125	20030916
AU 2003272896	A1	20040419	AU 2003-272896	20030926
EP 1555261	A1	20050720	EP 2003-753957	20030926
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
CN 1684949	A	20051019	CN 2003-823085	20030926
IN 2005CN00483	A	20070824	IN 2005-CN483	20050324
US 2006258559	A1	20061116	US 2005-529290	20050325
IN 2007CN01476	A	20070928	IN 2007-CN1476	20070412

PRIORITY APPLN. INFO.:		
JP 2002-282675	A	20020927
JP 2002-308952	A	20021023
JP 2003-323125	A	20030916
WO 2003-JP12341	W	20030926
IN 2005-CN483	A3	20050324

OTHER SOURCE(S): MARPAT 140:321236
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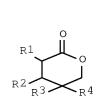

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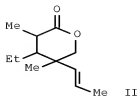

II

AB Disclosed are a valerolactone compound represented by the formula (I) (wherein R1 and R2 each independently represents hydrogen, Me, or ethyl; R3 represents hydrogen or methyl; and R4 represents Pr, 1-propenyl, or phenyl; provided that not both of R1 and R2 are hydrogen), in particular, the valerolactone compound represented by the formula (II), and a process for producing that compound, and a perfume composition containing any of the valerolactone compds. Compds. I are useful as perfume or flavor compns. for household products, cosmetics, public health products, beverages, and foods such as detergents, fabric softeners, shampoos, body cleansers, milk flavors, milk coffee, or perfumes. Thus, Michael addition reaction of 2-pentenenitrile with di-Me methylmalonate in the presence of NaOMe in methanol at 130° for 7 h and reduction of the resulting di-Me 2-methyl-2-[1-(cyanomethyl)propyl]malonate by LiBH4 in THF at 30° for 3 h gave 3-(cyanomethyl)-2-methyl-2-hydroxymethyl-1-pentanol which underwent hydrolysis in aqueous NaOH solution at 97° for 2.5 h and acidification with 6 N aqueous HCl solution to give 4-ethyl-5-(hydroxymethyl)-5- methyl-tetrahydropyran-2-one (III). Oxidation of III by pyridinium dichromate in CH2Cl2 at room temperature for 17 h and Wittig reaction of the resulting 4-ethyl-5-formyl-5-methyltetrahydropyran-2-one with ethyltriphenylphosphonium bromide using PhLi in hexane/THF gave 4-ethyl-5-methyl-5-(cis-1-propenyl)tetrahydropyran-2-one which underwent cis-trans isomerization in the presence of thiophenol and 2,2'-bisazobutyronitrile at 80° for 2 h to give 4-ethyl-5-methyl-5-(trans-1-propenyl)tetrahydropyran-2-one.

IC ICM C07D309-30
ICS A61K007-46; C11B009-00; A23L001-226; A23L002-00

CC 27-13 (Heterocyclic Compounds (One Hetero Atom))
Section cross-reference(s): 17, 62

L51 ANSWER 3 OF 11 ZCAPLUS COPYRIGHT 2008 ACS on STN DUPLICATE 3
ACCESSION NUMBER: 2000:765408 ZCAPLUS Full-text
DOCUMENT NUMBER: 133:321651
TITLE: Preparation of alkylcyclohexanones and their fragrance compositions
INVENTOR(S): Hashizume, Naomichio; Fukuda, Kazuyuki; Tanaka, Shigeyoshi; Koshino, Junji
PATENT ASSIGNEE(S): Kao Corp., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 5 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2000302722	A	20001031	JP 1999-115263	19990422
PRIORITY APPLN. INFO.:			JP 1999-115263	19990422

OTHER SOURCE(S): MARPAT 133:321651
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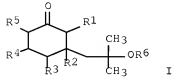

I

AB Alkylcyclohexanones I (R1-R6 = H, Me, Et; the total number of C in R1-R6 is ≤3) are prepared 2-Methyl-1-propenylmagnesium bromide was treated with 2-cyclohexenone, and the condensation product was hydrogenated by NaBH4, methoxylated, and oxidized with pyridinium chlorochromate to give 10% I (R1-R5 = H, R6 = Me). The product had floral, fruity, and green odor.
IC ICM C07C049-517
ICS A61K007-46; C11B009-00
CC 24-5 (Alicyclic Compounds)
Section cross-reference(s): 62
IT Odor and Odorous substances
Perfumes
(preparation of alkylcyclohexanones for fragrance compns.)

L51 ANSWER 4 OF 11 ZCAPLUS COPYRIGHT 2008 ACS on STN DUPLICATE 4
ACCESSION NUMBER: 2000:761945 ZCAPLUS Full-text
DOCUMENT NUMBER: 133:321648
TITLE: Preparation of cyclohexanols and their fragrance compositions
INVENTOR(S): Hashizume, Naomichio; Fukuda, Kazuyuki; Tanaka, Shigeyoshi; Koshino, Junji
PATENT ASSIGNEE(S): Kao Corp., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 7 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2000302713	A	20001031	JP 1999-115262	19990422

PRIORITY APPLN. INFO.: JP 1999-115262 19990422
OTHER SOURCE(S): MARPAT 133:321648
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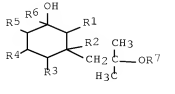

I

AB Cyclohexanols I (R1-R7 = H, Me, Et; the total number of C in R1-R7 is ≤3) are prepared 3-(2-Methylpropenyl)cyclohexanone was hydrogenated by NaBH4 at room temperature for 12 h in THF and the product was treated with MeOH and H2SO4 at -70° for 12 h to give 15% I (R1-R6 = H, R7 = Me). The product had floral, muguet, and sandalwood-like odor.
IC ICM C07C035-08
ICS C07C043-13; C11B009-00; C11D003-50; C11D009-44
CC 24-5 (Alicyclic Compounds)
IT Odor and Odorous substances
Perfumes
(preparation of cyclohexanols for fragrance compns.)

L51 ANSWER 5 OF 11 ZCAPLUS COPYRIGHT 2008 ACS on STN DUPLICATE 5
ACCESSION NUMBER: 2000:765402 ZCAPLUS Full-text
DOCUMENT NUMBER: 133:321650
TITLE: Preparation of cyclohexylmethanols and their fragrance compositions
INVENTOR(S): Hashizume, Naomichio; Fukuda, Kazuyuki; Tanaka, Shigeyoshi; Koshino, Junji
PATENT ASSIGNEE(S): Kao Corp., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 5 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2000302712	A	20001031	JP 1999-110760	19990419
PRIORITY APPLN. INFO.:			JP 1999-110760	19990419

OTHER SOURCE(S): MARPAT 133:321650
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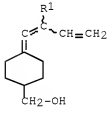

I

AB Cyclohexylmethanols I (R1 = H, Me; the broken line is an optional bond) are prepared Condensation of Me2CO with 4-hydroxymethylcyclohexanecarbaldeh yde gave the corresponding α,β-unsatd. ketone, which was hydrogenated with NaBH4 and dehydrated to afford 19% I (R1 = H). The product had floral and grapefruit-like odor.
IC ICM C07C033-14

ICS A61K007-46; C11B009-00; C11D003-50; C11D009-44
CC 24-5 (Alicyclic Compounds)
Section cross-reference(s): 62
IT Odor and Odorous substances
Perfumes
(preparation of cyclohexylmethanols for fragrance compns.)

L51 ANSWER 6 OF 11 ZCAPLUS COPYRIGHT 2008 ACS on STN DUPLICATE 6
ACCESSION NUMBER: 2000:408806 ZCAPLUS Full-text
DOCUMENT NUMBER: 133:30534
TITLE: Preparation of cyclohexylalkanols as perfume raw material
INVENTOR(S): Tanaka, Shigeyoshi; Yamamoto, Junko; Koshino, Junji; Fukuda, Kazuyuki; Toi, Naoshi
PATENT ASSIGNEE(S): Kao Corp., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 6 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2000169409	A	20000620	JP 1998-345611	19981204
JP 3756332	B2	20060315		
PRIORITY APPLN. INFO.:			JP 1998-345611	19981204
OTHER SOURCE(S):	MARPAT 133:30534			

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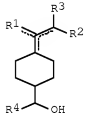

I

AB The title compds. (I; R1, R2, R3, R4 = H, Me, or Et and a total number of carbon atoms in R1-R4 is 2-3; a single line accompanied by a parallel dotted line appearing in three locations each represent a single or a double bond and one of these bonds represent a double bond.) are prepared These compds. possess floral fragrance and are useful as perfume components for toiletries. Thus, isopropyltriphenylphosphonium iodide was treated with potassium tert-butoxide in THF at room temperature for 1 h, and cooled in ice, followed by adding a solution of 4-(tetrahydropyran-2-yloxymethyl)cyclohexanecarboxaldehyde (preparation given) in THF, and the resulting mixture was stirred at 25° for 4 h to give, after deprotection of tetrahydropyranyl group by p-MeC6H4SO3H in MeOH, title compound (II).
IC ICM C07C033-14
ICS A61K007-46; C11B009-00
CC 24-5 (Alicyclic Compounds)
Section cross-reference(s): 62

ST cyclohexylalkanol prepn perfume
IT Odor and Odorous substances
Perfumes
(preparation of cyclohexylalkanols as perfume raw material)
IT 273735-14-1P 273735-16-3P 273735-17-4P 273933-07-6P 273933-08-7P
RL: BSU (Biological study, unclassified); BUU (Biological use, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of cyclohexylalkanols as perfume raw material)
IT 78-93-3, Methyl ethyl ketone, reactions 110-87-2, Dihydropyran 873-75-6, p-Bromobenzyl alcohol 4762-30-5, sec-Butyltriphenylphosphonium iodide 5391-88-8 14350-50-6, n-Propyltriphenylphosphonium iodide 24470-78-8, Isopropyltriphenylphosphonium iodide 92385-32-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of cyclohexylalkanols as perfume raw material)
IT 17100-68-4P 273735-13-0P 273735-15-2P 273735-18-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of cyclohexylalkanols as perfume raw material)

L51 ANSWER 7 OF 11 ZCAPLUS COPYRIGHT 2008 ACS on STN DUPLICATE 7
ACCESSION NUMBER: 1999:182540 ZCAPLUS Full-text
DOCUMENT NUMBER: 130:271888
TITLE: Cyclohexylalkanols and fragrance compositions containing them
INVENTOR(S): Tanaka, Shigeyoshi; Yamamoto, Junko; Koshino, Junji; Fukuda, Kazuyuki; Toi, Naoshi
PATENT ASSIGNEE(S): Kao Corp., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 11 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 11071312	A	19990316	JP 1997-230792	19970827
JP 4027471	B2	20071226		
PRIORITY APPLN. INFO.:			JP 1997-230792	19970827
OTHER SOURCE(S):	MARPAT	130:271888		

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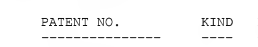

I

AB Fragrance compns., which show long-lasting fragrance, contain title compds. I (R1-R4 = C1-3 alkyl, H; R5 = C1-3 alkyl). 4-Bromobenzyl alc. was etherified with MeI in THF in the presence of NaH, converted into Grignard reagent, treated with MeCHO in THF at room temperature for 12 h, and reduced by H in i-PrOH using Ru/C at 90° under 0.5 MPa for 3 days to give 38% I (R1 = R5 = Me, R2-R4 = H), which showed woody, floral, and muguet-like fragrance for 4 days.
IC ICM C07C043-13
ICS C11B009-00
CC 62-5 (Essential Oils and Cosmetics)

Section cross-reference(s): 24
IT Perfumes
(preparation of cyclohexylalkanols for fragrance compns.)

L51 ANSWER 8 OF 11 ZCAPLUS COPYRIGHT 2008 ACS on STN DUPLICATE 8
ACCESSION NUMBER: 1999:107143 ZCAPLUS Full-text
DOCUMENT NUMBER: 130:213502
TITLE: Perfume compositions containing 4-alkoxymethylcyclohexylmethanols
INVENTOR(S): Tanaka, Shigeyoshi; Yamamoto, Junko; Koshino, Junji; Toi, Tadashi; Fukuda, Kazuyuki
PATENT ASSIGNEE(S): Kao Corp., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 5 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 11035969	A	19990209	JP 1997-188069	19970714
JP 3833347	B2	20061011		
PRIORITY APPLN. INFO.:			JP 1997-188069	19970714
OTHER SOURCE(S):	MARPAT 130:213502			

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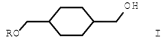

I

AB The compns. contain the title compds. I (R = C1-10 alkyl, C3-10 cycloalkyl, C2-10 alkenyl). The compns. have stable fragrance like lily of the valley. A floral fragrance for detergents was formulated from hexylcinnamic aldehyde 200, phenylethylalc. 200, rhodinol 200, citronellol 150, hydroxycitronellal 50, and I (R = Et) (preparation given) 200 parts.
IC ICM C11B009-00
ICS A61K007-00; A61K007-46; A61K007-50
CC 62-5 (Essential Oils and Cosmetics)
ST floral perfume alkoxymethylcyclohexylmethanol prepn; cyclohexylmethanol alkoxymethyl prepn floral perfume
IT Cosmetics
Detergents
Perfumes
(preparation of 4-alkoxymethylcyclohexylmethanols having fragrance like lily
of the valley and perfume compns. containing them)
IT 33424-86-1P, 4-Allyloxymethylcyclohexylmethanol 98955-27-2P, 4-Methoxymethylcyclohexylmethanol 220331-53-3P, 4-Ethoxymethylcyclohexylmethanol 220331-54-4P, 4-Isopropoxymethylcyclohexylmethanol
RL: BUU (Biological use, unclassified); PNU (Preparation, unclassified); TEM (Technical or engineered material use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of 4-alkoxymethylcyclohexylmethanols having fragrance like

lily
of the valley and perfume compns. containing them)
IT 74-88-4, Methyl iodide, reactions 74-96-4, Ethyl bromide 75-30-9, 2-Iodopropane 105-08-8, 1,4-Dimethylolcyclohexane 556-56-9, Allyl iodide
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of 4-alkoxymethylcyclohexylmethanols having fragrance like lily
of the valley and perfume compns. containing them)

L51 ANSWER 9 OF 11 ZCAPLUS COPYRIGHT 2008 ACS on STN DUPLICATE 9
ACCESSION NUMBER: 1998:485420 ZCAPLUS Full-text
DOCUMENT NUMBER: 129:179988
TITLE: 2,2-Dimethyl-3-alkoxypropanols and fragrance compositions containing these
INVENTOR(S): Tanaka, Shigeyoshi; Koshino, Junji; Fukuda, Kazuyuki; Toi, Naoshi
PATENT ASSIGNEE(S): Kao Corp., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 5 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 10195010	A	19980728	JP 1997-577	19970107
PRIORITY APPLN. INFO.:			JP 1997-577	19970107

OTHER SOURCE(S): MARPAT 129:179988
AB Fragrance compns. contain HOCH2CMe2CH2OCH2R (R = C3-6 branched alkyl). Acid-catalyzed cyclization of isobutyraldehyde with 2,2-dimethyl-1,3- propanediol to give a 1,3-dioxane derivative followed by reduction with diisobutylaluminum hydride gave 2,2-dimethyl-3-(2-methylpropyloxy)-1- propanol, which showed floral odor.
IC ICM C07C043-13
ICS C11B009-00
CC 62-5 (Essential Oils and Cosmetics)
Section cross-reference(s): 23
ST methylalkoxypropanol prepn perfume; propanol methylalkoxy prepn perfume; fragrance dimethylalkoxypropanol prepn
IT Perfumes
(preparation of 2,2-dimethyl-3-alkoxypropanols for fragrance compns.)

L51 ANSWER 10 OF 11 ZCAPLUS COPYRIGHT 2008 ACS on STN DUPLICATE 10
ACCESSION NUMBER: 1997:416661 ZCAPLUS Full-text
DOCUMENT NUMBER: 127:55670
TITLE: Perfumes containing 4-(2-methoxyphenyl)-2-methyl-2-butanol
INVENTOR(S): Tanaka, Shigeyoshi; Etsuno, Junji; Fukuda, Kazuyuki; Toi, Sunao
PATENT ASSIGNEE(S): Kao Corp., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 4 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE

JP 09111281	A	19970428	JP 1995-270893	19951019
JP 3462319	B2	20031105		

PRIORITY APPLN. INFO.: JP 1995-270893 19951019

AB The title compound with flowery scent is prepared and formulated with other aromatic compds. for cosmetics and perfumes.

IC ICM C11B009-00
ICS C11D003-50

CC 62-5 (Essential Oils and Cosmetics)

ST methoxyphenylmethylbutanol prepn perfume

IT Perfumes
(perfumes containing 4-(2-methoxyphenyl)-2-methyl-2-butanol)

IT 56052-48-3P
RL: BUU (Biological use, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(perfumes containing 4-(2-methoxyphenyl)-2-methyl-2-butanol)

IT 105-36-2, Ethyl bromoacetate 135-02-4, o-Anisaldehyde
RL: RCT (Reactant); RACT (Reactant or reagent)
(perfumes containing 4-(2-methoxyphenyl)-2-methyl-2-butanol)

IT 70200-18-9P 70311-27-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(perfumes containing 4-(2-methoxyphenyl)-2-methyl-2-butanol)

L51 ANSWER 11 OF 11 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2006:142819 ZCAPLUS Full-text
DOCUMENT NUMBER: 144:232917
TITLE: Preparation of novel pyrans and perfume compositions containing them
INVENTOR(S): Asada, Takahiro; Tanaka, Shigeyoshi
PATENT ASSIGNEE(S): Kao Corp., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 11 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2006045111	A	20060216	JP 2004-228018	20040804

PRIORITY APPLN. INFO.: JP 2004-228018 20040804
OTHER SOURCE(S): MARPAT 144:232917
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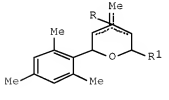

I

AB Pyrans I (R = H, OH; when R = H, then 1 of the broken lines may be double bond; when R = OH; all the broken lines = single bonds; R1 = H, Me) are

prepared by cyclization of 2,4,6-trimethylbenzaldehyde (II) with H2C:CMeCH2CHR1OH (R1 = same as above) in the presence of acid catalysts. Thus, II was treated with isoprenol and p-toluenesulfonic acid at 100°C for 3 h to give I (R = R1 = H; 1 of the broken lines is double bond) and I (R = R1 = H; all the broken lines = single bonds), which possessed herbal odor and sweet odor, resp.

CC 27-13 (Heterocyclic Compounds (One Hetero Atom))
Section cross-reference(s): 62

ST trimethylphenyl pyran prepn perfume; trimethylbenzaldehyde cyclization isoprenol toluenesulfonic acid catalyst

IT Cyclocondensation reaction catalysts
Perfumes
(preparation of (trimethylphenyl)pyrans for perfume compns.)

IT Acids, uses
RL: CAT (Catalyst use); USES (Uses)
(preparation of (trimethylphenyl)pyrans for perfume compns.)

IT 104-15-4, p-Toluenesulfonic acid, uses
RL: CAT (Catalyst use); USES (Uses)
(preparation of (trimethylphenyl)pyrans for perfume compns.)

IT 876132-59-1P
RL: COS (Cosmetic use); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of (trimethylphenyl)pyrans for perfume compns.)

IT 876132-58-0P 876132-60-4P 876132-61-5P 876132-62-6P 876132-63-7P 876132-64-8P
RL: COS (Cosmetic use); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of (trimethylphenyl)pyrans for perfume compns.)

IT 487-68-3, 2,4,6-Trimethylbenzaldehyde 763-32-6, Isoprenol 2004-67-3, 4-Methyl-4-penten-2-ol
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of (trimethylphenyl)pyrans for perfume compns.)

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(COVERAGE TO THESE DATES IS NOT COMPLETE):

US 20080329170 7 FEB 2008
DE 102006035202 31 JAN 2008
EP 1882693 30 JAN 2008
JP 2008024674 07 FEB 2008
WO 2008021152 21 FEB 2008
GB 2439172 19 DEC 2007
FR 2904316 01 FEB 2008
RU 2316552 10 FEB 2008
CA 2593150 06 JAN 2008

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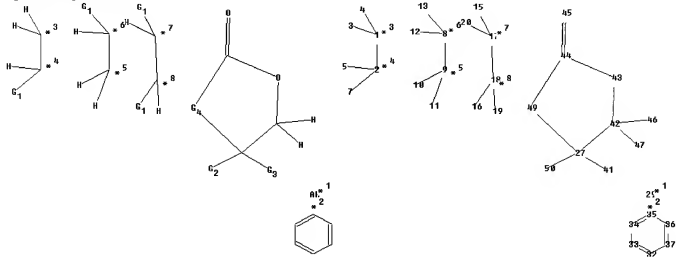

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ring bonds :
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44
44-49
exact/norm bonds :
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42-46  42-47  44-45
exact bonds :
1-2  8-9  17-18  27-49  27-42  42-43  43-44  44-49
normalized bonds :
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G1:CH3,Et

G2:CH3,H

G3:[*1],[*2]

G4:[*3-*4],[*5-*6],[*7-*8]
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11:CLASS
12:CLASS  13:CLASS  15:CLASS  16:CLASS  17:Atom  18:Atom  19:CLASS  20:CLASS
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Element Count :
Node 29: Limited
    C,C3



L24          96 SEA FILE=MARPAT SSS FUL L1
L25             STR

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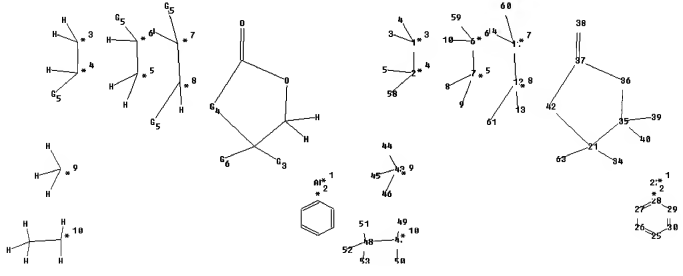

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chain bonds :
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ring bonds :
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37
37-42
exact/norm bonds :
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35-39 35-40 37-38 43-44 43-45 43-46 47-48 47-49 47-50 48-51 48-52 48-53
exact bonds :
1-2 6-7 11-12 21-42 21-35 35-36 36-37 37-42
normalized bonds :
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G3:[*1],[*2]

G4:[*3-*4],[*5-*6],[*7-*8]

G5:[*9],[*10]

G6:H,[*9]

Connectivity :
22:1 E exact RC ring/chain
Match level :
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10:CLASS
11:Atom 12:Atom 13:CLASS 14:CLASS 21:Atom 22:Atom 25:Atom 26:Atom 27:Atom
28:Atom 29:Atom
30:Atom 34:CLASS 35:Atom 36:Atom 37:Atom 38:Atom 39:CLASS 40:CLASS 42:Atom
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52:CLASS 53:CLASS
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Element Count :
Node 22: Limited
C,C3

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9"/AN)
L48 1 SEA FILE=MARPAT ABB=ON PLU=ON L47 AND L27

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=> d ibib abs qhit 1 L48

L48 ANSWER 1 OF 1 MARPAT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 140:321236 MARPAT Full-text
TITLE: Preparation of valerolactone compounds and perfume
composition
INVENTOR(S): Tanaka, Sakuya; Fukuda, Kazuyuki; Asada, Takahiro
PATENT ASSIGNEE(S): Kao Corporation, Japan
SOURCE: PCT Int. Appl., 65 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004029033	A1	20040408	WO 2003-JP12341	20030926
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
JP 2004161746	A	20040610	JP 2003-323125	20030916
AU 2003272896	A1	20040419	AU 2003-272896	20030926
EP 1555261	A1	20050720	EP 2003-753957	20030926
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CN 1684949	A	20051019	CN 2003-823085	20030926
IN 2005CN00483	A	20070824	IN 2005-CN483	20050324
US 2006258559	A1	20061116	US 2005-529290	20050325
IN 2007CN01476	A	20070928	IN 2007-CN1476	20070412

PRIORITY APPLN. INFO.:

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JP 2002-308952 20021023
JP 2003-323125 20030916
WO 2003-JP12341 20030926
IN 2005-CN483 20050324

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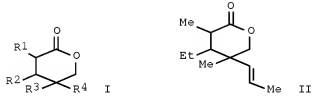

AB Disclosed are a valerolactone compound represented by the formula (I) (wherein R1 and R2 each independently represents hydrogen, Me, or ethyl; R3 represents hydrogen or methyl; and R4 represents Pr, 1-propenyl, or phenyl; provided that not both of R1 and R2 are hydrogen), in particular, the valerolactone compound represented by the formula (II), and a process for producing that compound, and a perfume composition containing any of the valerolactone compds. Compds. I are useful as perfume or flavor compns. for household products, cosmetics, public health products, beverages, and foods such as detergents, fabric softeners, shampoos, body cleansers, milk flavors, milk coffee, or perfumes. Thus, Michael addition reaction of 2-pentenenitrile with di-Me methylmalonate in the presence of NaOMe in methanol at 130° for 7 h and reduction of the resulting di-Me 2-methyl-2-[1-(cyanomethyl)propyl]malonate by LiBH4 in THF at 30° for 3 h gave 3-(cyanomethyl)-2-methyl-2-hydroxymethyl-1-pentanol which

underwent hydrolysis in aqueous NaOH solution at 97° for 2.5 h and acidification with 6 N aqueous HCl solution to give 4-ethyl-5-(hydroxymethyl)-5- methyl-tetrahydropyran-2-one (III). Oxidation of III by pyridinium dichromate in CH2Cl2 at room temperature for 17 h and Wittig reaction of the resulting 4-ethyl-5-formyl-5-methyltetrahydropyran-2-one with ethyltriphenylphosphonium bromide using PhLi in hexane/THF gave 4-ethyl-5-methyl-5-(cis-1-propenyl)tetrahydropyran-2-one which underwent cis-trans isomerization in the presence of thiophenol and 2,2'-bisazobutyronitrile at 80° for 2 h to give 4-ethyl-5-methyl-5-(trans-1-propenyl)tetrahydropyran-2-one.

MSTR 1

G1 = Me
G3 = Pr-n
Patent location: claim 1

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DICTIONARY FILE UPDATES:  25 MAR 2008  HIGHEST RN 1010115-69-1

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=> d stat que L14
L1              STR

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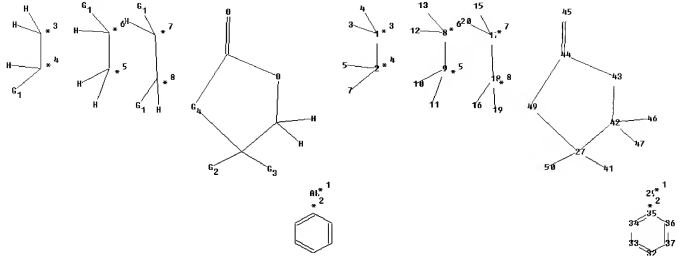

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42-46  42-47  44-45
ring bonds :
1-2  8-9  17-18  27-49  27-42  32-33  32-37  33-34  34-35  35-36  36-37  42-43  43-
44
44-49
exact/norm bonds :
1-3  1-4  2-5  2-7  8-12  8-13  9-10  9-11  15-17  16-18  17-20  18-19  27-41  27-
50
42-46  42-47  44-45
exact bonds :
1-2  8-9  17-18  27-49  27-42  42-43  43-44  44-49
normalized bonds :
32-33  32-37  33-34  34-35  35-36  36-37


G1:CH3,Et

G2:CH3,H

G3:[*1],[*2]

G4:[*3-*4],[*5-*6],[*7-*8]

Connectivity :
29:1 E exact RC ring/chain
Match level :
1:Atom  2:Atom  3:CLASS  4:CLASS  5:CLASS  7:CLASS  8:Atom  9:Atom  10:CLASS
11:CLASS
12:CLASS  13:CLASS  15:CLASS  16:CLASS  17:Atom  18:Atom  19:CLASS  20:CLASS
27:Atom  29:CLASS
32:Atom  33:Atom  34:Atom  35:Atom  36:Atom  37:Atom  41:CLASS  42:Atom  43:Atom
44:Atom  45:CLASS
46:CLASS  47:CLASS  49:Atom  50:CLASS
```

```
Element Count :
Node 29: Limited
    C,C3

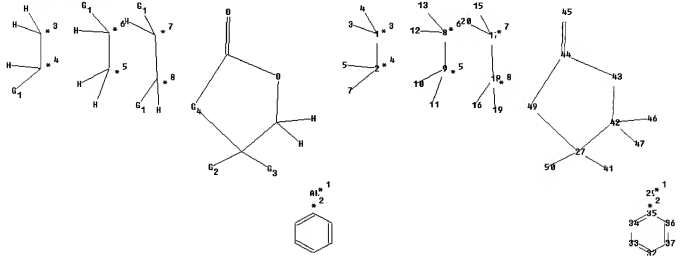


L9            16 SEA FILE=REGISTRY SSS FUL L1
L14            7 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  L9


=> d stat que L15
L1              STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY -  AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation:
Uploading L1.str
```



```
chain nodes :
3  4  5  7  10  11  12  13  15  16  19  20  29  41  45  46  47  50
ring nodes :
1  2  8  9  17  18  27  32  33  34  35  36  37  42  43  44  49
chain bonds :
1-3  1-4  2-5  2-7  8-12  8-13  9-10  9-11  15-17  16-18  17-20  18-19  27-41  27-
50
42-46  42-47  44-45
ring bonds :
1-2  8-9  17-18  27-49  27-42  32-33  32-37  33-34  34-35  35-36  36-37  42-43  43-
44
44-49
exact/norm bonds :
1-3  1-4  2-5  2-7  8-12  8-13  9-10  9-11  15-17  16-18  17-20  18-19  27-41  27-
50
42-46  42-47  44-45
exact bonds :
1-2  8-9  17-18  27-49  27-42  42-43  43-44  44-49
normalized bonds :
32-33  32-37  33-34  34-35  35-36  36-37
```

```
G1:CH3,Et

G2:CH3,H

G3:[*1],[*2]

G4:[*3-*4],[*5-*6],[*7-*8]

Connectivity :
29:1 E exact RC ring/chain
Match level :
1:Atom  2:Atom  3:CLASS  4:CLASS  5:CLASS  7:CLASS  8:Atom  9:Atom  10:CLASS
11:CLASS
12:CLASS  13:CLASS  15:CLASS  16:CLASS  17:Atom  18:Atom  19:CLASS  20:CLASS
27:Atom  29:CLASS
32:Atom  33:Atom  34:Atom  35:Atom  36:Atom  37:Atom  41:CLASS  42:Atom  43:Atom
44:Atom  45:CLASS
46:CLASS  47:CLASS  49:Atom  50:CLASS
Element Count :
Node 29: Limited
    C,C3

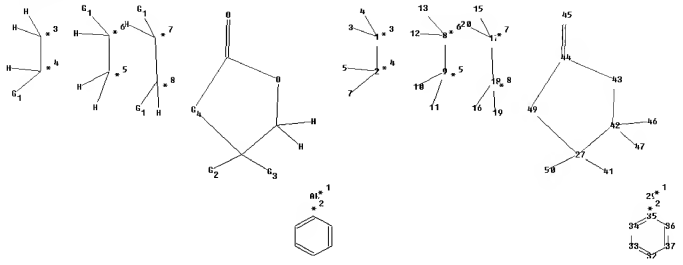



L6           32 SEA FILE=REGISTRY ABB=ON  PLU=ON  (107898-54-4/BI OR 123-38-6/B
                I OR 126-98-7/BI OR 13284-42-9/BI OR 1530-32-1/BI OR 23727-15-3
                /BI OR 28219-60-5/BI OR 28219-61-6/BI OR 609-02-9/BI OR
                623-36-9/BI OR 65113-99-7/BI OR 677326-31-7/BI OR 677326-32-8/B
                I OR 677326-33-9/BI OR 677326-34-0/BI OR 677326-35-1/BI OR
                677326-36-2/BI OR 677326-37-3/BI OR 677326-38-4/BI OR 677326-39
                -5/BI OR 677326-40-8/BI OR 677326-41-9/BI OR 677326-42-0/BI OR
                677326-43-1/BI OR 677326-44-2/BI OR 677326-45-3/BI OR 677326-46
                -4/BI OR 677763-76-7/BI OR 677763-77-8/BI OR 67801-20-1/BI OR
                72089-08-8/BI OR 93-53-8/BI)
L7           14 SEA FILE=REGISTRY ABB=ON  PLU=ON  L6 AND OC5/ES
L9           16 SEA FILE=REGISTRY SSS FUL L1
L10           9 SEA FILE=REGISTRY ABB=ON  PLU=ON  L9 AND L7
L11           5 SEA FILE=REGISTRY ABB=ON  PLU=ON  L7 NOT L10
L12        6097 SEA FILE=REGISTRY ABB=ON  PLU=ON  C10H18O2/MF
L13           1 SEA FILE=REGISTRY ABB=ON  PLU=ON  L11 AND L12
L14           7 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  L9
L15           1 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  L13 AND L14


=> d stat que L16
L1              STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY -  AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation:
Uploading L1.str
```



```
chain nodes :
3  4  5  7  10  11  12  13  15  16  19  20  29  41  45  46  47  50
ring nodes :
1  2  8  9  17  18  27  32  33  34  35  36  37  42  43  44  49
chain bonds :
1-3  1-4  2-5  2-7  8-12  8-13  9-10  9-11  15-17  16-18  17-20  18-19  27-41  27-
50
42-46  42-47  44-45
ring bonds :
1-2  8-9  17-18  27-49  27-42  32-33  32-37  33-34  34-35  35-36  36-37  42-43  43-
44
44-49
exact/norm bonds :
1-3  1-4  2-5  2-7  8-12  8-13  9-10  9-11  15-17  16-18  17-20  18-19  27-41  27-
50
42-46  42-47  44-45
exact bonds :
1-2  8-9  17-18  27-49  27-42  42-43  43-44  44-49
normalized bonds :
32-33  32-37  33-34  34-35  35-36  36-37


G1:CH3,Et

G2:CH3,H

G3:[*1],[*2]

G4:[*3-*4],[*5-*6],[*7-*8]

Connectivity :
29:1 E exact RC ring/chain
Match level :
1:Atom  2:Atom  3:CLASS  4:CLASS  5:CLASS  7:CLASS  8:Atom  9:Atom  10:CLASS
11:CLASS
12:CLASS  13:CLASS  15:CLASS  16:CLASS  17:Atom  18:Atom  19:CLASS  20:CLASS
27:Atom  29:CLASS
32:Atom  33:Atom  34:Atom  35:Atom  36:Atom  37:Atom  41:CLASS  42:Atom  43:Atom
44:Atom  45:CLASS
46:CLASS  47:CLASS  49:Atom  50:CLASS
Element Count :
```

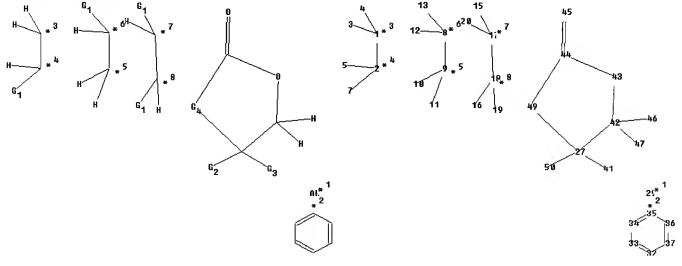
Node 29: Limited
C,C3

L6 32 SEA FILE=REGISTRY ABB=ON PLU=ON (107898-54-4/BI OR 123-38-6/BI OR 126-98-7/BI OR 13284-42-9/BI OR 1530-32-1/BI OR 23727-15-3/BI OR 28219-60-5/BI OR 28219-61-6/BI OR 609-02-9/BI OR 623-36-9/BI OR 65113-99-7/BI OR 677326-31-7/BI OR 677326-32-8/BI OR 677326-33-9/BI OR 677326-34-0/BI OR 677326-35-1/BI OR 677326-36-2/BI OR 677326-37-3/BI OR 677326-38-4/BI OR 677326-39-5/BI OR 677326-40-8/BI OR 677326-41-9/BI OR 677326-42-0/BI OR 677326-43-1/BI OR 677326-44-2/BI OR 677326-45-3/BI OR 677326-46-4/BI OR 677763-76-7/BI OR 677763-77-8/BI OR 67801-20-1/BI OR 72089-08-8/BI OR 93-53-8/BI)
L9 16 SEA FILE=REGISTRY SSS FUL L1
L14 7 SEA FILE=ZCAPLUS ABB=ON PLU=ON L9
L16 2 SEA FILE=ZCAPLUS ABB=ON PLU=ON L6 AND L14

=> d stat que L33
L1 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation:
Uploading L1.str



chain nodes :
3 4 5 7 10 11 12 13 15 16 19 20 29 41 45 46 47 50
ring nodes :
1 2 8 9 17 18 27 32 33 34 35 36 37 42 43 44 49
chain bonds :
1-3 1-4 2-5 2-7 8-12 8-13 9-10 9-11 15-17 16-18 17-20 18-19 27-41 27-50
42-46 42-47 44-45
ring bonds :
1-2 8-9 17-18 27-49 27-42 32-33 32-37 33-34 34-35 35-36 36-37 42-43 43-44

```
44-49
exact/norm bonds :
1-3  1-4  2-5  2-7  8-12  8-13  9-10  9-11  15-17  16-18  17-20  18-19  27-41  27-
50
42-46  42-47  44-45
exact bonds :
1-2  8-9  17-18  27-49  27-42  42-43  43-44  44-49
normalized bonds :
32-33  32-37  33-34  34-35  35-36  36-37


G1:CH3,Et

G2:CH3,H

G3:[*1],[*2]

G4:[*3-*4],[*5-*6],[*7-*8]

Connectivity :
29:1 E exact RC ring/chain
Match level :
1:Atom  2:Atom  3:CLASS  4:CLASS  5:CLASS  7:CLASS  8:Atom  9:Atom  10:CLASS
11:CLASS
12:CLASS  13:CLASS  15:CLASS  16:CLASS  17:Atom  18:Atom  19:CLASS  20:CLASS
27:Atom  29:CLASS
32:Atom  33:Atom  34:Atom  35:Atom  36:Atom  37:Atom  41:CLASS  42:Atom  43:Atom
44:Atom  45:CLASS
46:CLASS  47:CLASS  49:Atom  50:CLASS
Element Count :
Node 29: Limited
    C,C3

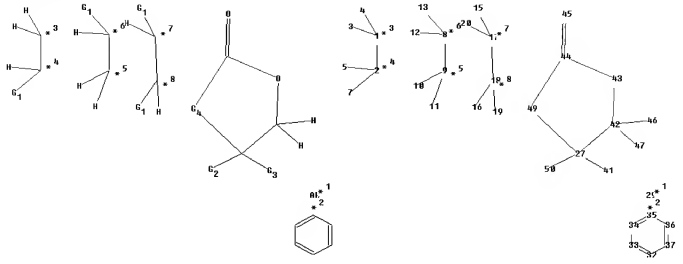



L9            16 SEA FILE=REGISTRY SSS FUL L1
L33            1 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  L9 (L) COS/RL


=> d stat que L34
L1              STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY -  AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation:
Uploading L1.str
```



```
chain nodes :
3  4  5  7  10  11  12  13  15  16  19  20  29  41  45  46  47  50
ring nodes :
1  2  8  9  17  18  27  32  33  34  35  36  37  42  43  44  49
chain bonds :
1-3  1-4  2-5  2-7  8-12  8-13  9-10  9-11  15-17  16-18  17-20  18-19  27-41  27-
50
42-46  42-47  44-45
ring bonds :
1-2  8-9  17-18  27-49  27-42  32-33  32-37  33-34  34-35  35-36  36-37  42-43  43-
44
44-49
exact/norm bonds :
1-3  1-4  2-5  2-7  8-12  8-13  9-10  9-11  15-17  16-18  17-20  18-19  27-41  27-
50
42-46  42-47  44-45
exact bonds :
1-2  8-9  17-18  27-49  27-42  42-43  43-44  44-49
normalized bonds :
32-33  32-37  33-34  34-35  35-36  36-37


G1:CH3,Et

G2:CH3,H

G3:[*1],[*2]

G4:[*3-*4],[*5-*6],[*7-*8]

Connectivity :
29:1 E exact RC ring/chain
Match level :
1:Atom  2:Atom  3:CLASS  4:CLASS  5:CLASS  7:CLASS  8:Atom  9:Atom  10:CLASS
11:CLASS
12:CLASS  13:CLASS  15:CLASS  16:CLASS  17:Atom  18:Atom  19:CLASS  20:CLASS
27:Atom  29:CLASS
32:Atom  33:Atom  34:Atom  35:Atom  36:Atom  37:Atom  41:CLASS  42:Atom  43:Atom
44:Atom  45:CLASS
46:CLASS  47:CLASS  49:Atom  50:CLASS
Element Count :
```

```
Node 29: Limited
    C,C3



L9            16 SEA FILE=REGISTRY SSS FUL L1
L14            7 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  L9
L31        89969 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  COSME?/BI
L32        36798 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  ?PERFUM?/BI
L34            1 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  L14 AND (L31 OR L32)


=> s L14-L16 or L33-L34
L52            7 (L14 OR L15 OR L16) OR (L33 OR L34)

=> s L52 not L38,L43
L53            6 L52 NOT (L38 OR L43)

=> file beilstein
FILE 'BEILSTEIN' ENTERED AT 16:59:48 ON 26 MAR 2008
COPYRIGHT (c) 2008 Beilstein-Institut zur Foerderung der Chemischen Wissenschaften
licensed to Beilstein GmbH and MDL Information Systems GmbH

FILE LAST UPDATED ON January 3, 2008

FILE COVERS 1771 TO 2007.
*** FILE CONTAINS 10.119,480  SUBSTANCES ***

>>>PLEASE NOTE: Reaction Data and substance data are stored in
   separate documents and can not be searched together in one query.
   Reaction data for BEILSTEIN compounds may be displayed
   immediately with the display codes PRE (preparations) and REA
   (reactions).  A substance answer set retrieved after the search
   for a chemical name, a compounds with available reaction
   information by combining with PRE/FA, REA/FA or more generally
   with RX/FA. The BEILSTEIN Registry Number (BRN) is the link
   between a BEILSTEIN compound and belonging reactions. For mo
   detailed reaction searches BRNs can be searched as reaction
   partner BRNs Reactant BRN (RX.RBRN) or Product BRN (RX.PBRN).<<<

>>> FOR SEARCHING PREPARATIONS SEE HELP PRE  <<<

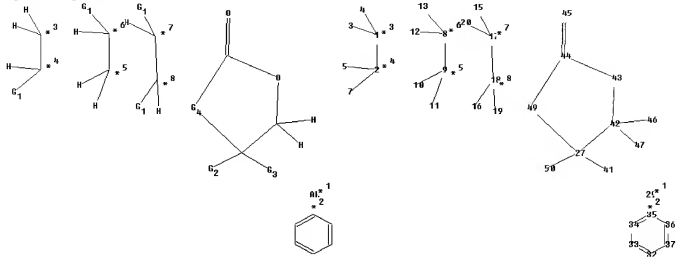
**********************************************************************
* PLEASE NOTE THAT THERE ARE NO FORMATS FREE OF COST.                *
* SET NOTICE FEATURE: THE COST ESTIMATES CALCULATED FOR SET NOTICE   *
* ARE BASED ON THE HIGHEST PRICE CATEGORY. THEREFORE; THESE          *
* ESTIMATES MAY NOT REFLECT THE ACTUAL COSTS.                        *
* FOR PRICE INFORMATION SEE HELP COST                                *
**********************************************************************

>>> Price change as of January 1st, 2008: Connect Time and Structure
    Search fees re-introduced. See NEWS and HELP COST <<<

=> d stat que L21
L1             STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY -  AVAILABLE VIA OFFLINE PRINT *
```

Structure attributes must be viewed using STN Express query preparation:
Uploading L1.str



chain nodes :
3 4 5 7 10 11 12 13 15 16 19 20 29 41 45 46 47 50
ring nodes :
1 2 8 9 17 18 27 32 33 34 35 36 37 42 43 44 49
chain bonds :
1-3 1-4 2-5 2-7 8-12 8-13 9-10 9-11 15-17 16-18 17-20 18-19 27-41 27-50
42-46 42-47 44-45
ring bonds :
1-2 8-9 17-18 27-49 27-42 32-33 32-37 33-34 34-35 35-36 36-37 42-43 43-44
44-49
exact/norm bonds :
1-3 1-4 2-5 2-7 8-12 8-13 9-10 9-11 15-17 16-18 17-20 18-19 27-41 27-50
42-46 42-47 44-45
exact bonds :
1-2 8-9 17-18 27-49 27-42 42-43 43-44 44-49
normalized bonds :
32-33 32-37 33-34 34-35 35-36 36-37

G1:CH3,Et

G2:CH3,H

G3:[*1],[*2]

G4:[*3-*4],[*5-*6],[*7-*8]

Connectivity :
29:1 E exact RC ring/chain
Match level :
1:Atom 2:Atom 3:CLASS 4:CLASS 5:CLASS 7:CLASS 8:Atom 9:Atom 10:CLASS 11:CLASS
12:CLASS 13:CLASS 15:CLASS 16:CLASS 17:Atom 18:Atom 19:CLASS 20:CLASS
27:Atom 29:CLASS
32:Atom 33:Atom 34:Atom 35:Atom 36:Atom 37:Atom 41:CLASS 42:Atom 43:Atom

```
44:Atom  45:CLASS
46:CLASS  47:CLASS  49:Atom  50:CLASS
Element Count :
Node 29: Limited
    C,C3




L19             SCR 1338
L21           4 SEA FILE=BEILSTEIN SSS FUL L1 AND L19

100.0% PROCESSED  145067 ITERATIONS                              4 ANSWERS
SEARCH TIME: 00.01.35



=> file marpat
FILE 'MARPAT' ENTERED AT 17:00:01 ON 26 MAR 2008
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2008 American Chemical Society (ACS)

FILE CONTENT: 1961-PRESENT VOL 148 ISS 11 (20080321/ED)

SOME MARPAT RECORDS ARE DERIVED FROM INPI DATA FOR 1961-1987

MOST RECENT CITATIONS FOR PATENTS FROM MAJOR ISSUING AGENCIES
(COVERAGE TO THESE DATES IS NOT COMPLETE):

US   2008032917 07 FEB 2008
DE 102006035202 31 JAN 2008
EP      1882693 30 JAN 2008
JP   2008024674 07 FEB 2008
WO   2008021152 21 FEB 2008
GB      2439172 19 DEC 2007
FR      2904316 01 FEB 2008
RU      2316552 10 FEB 2008
CA      2593150 06 JAN 2008

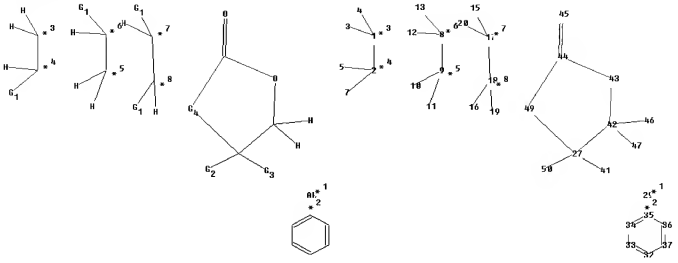
Expanded G-group definition display now available.

Effective December 15th the iteration and answer limits in MARPAT
have increased from 100,000 to 200,000 for both on-line and batch
searches.  For more information on MARPAT search limits, type HELP
SLIMITS at an arrow prompt.

=> d stat que L27
L1              STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY -  AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation:
Uploading L1.str
```



```
chain nodes :
3  4  5  7  10  11  12  13  15  16  19  20  29  41  45  46  47  50
ring nodes :
1  2  8  9  17  18  27  32  33  34  35  36  37  42  43  44  49
chain bonds :
1-3  1-4  2-5  2-7  8-12  8-13  9-10  9-11  15-17  16-18  17-20  18-19  27-41  27-
50
42-46  42-47  44-45
ring bonds :
1-2  8-9  17-18  27-49  27-42  32-33  32-37  33-34  34-35  35-36  36-37  42-43  43-
44
44-49
exact/norm bonds :
1-3  1-4  2-5  2-7  8-12  8-13  9-10  9-11  15-17  16-18  17-20  18-19  27-41  27-
50
42-46  42-47  44-45
exact bonds :
1-2  8-9  17-18  27-49  27-42  42-43  43-44  44-49
normalized bonds :
32-33  32-37  33-34  34-35  35-36  36-37


G1:CH3,Et

G2:CH3,H

G3:[*1],[*2]

G4:[*3-*4],[*5-*6],[*7-*8]

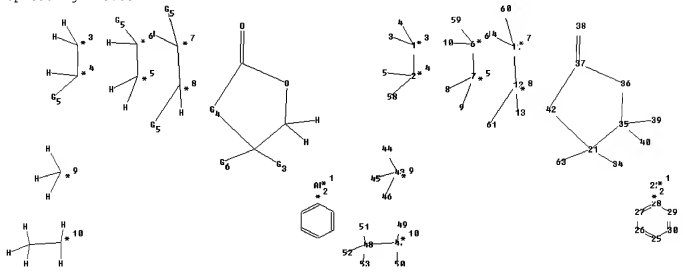
Connectivity :
29:1 E exact RC ring/chain
Match level :
1:Atom  2:Atom  3:CLASS  4:CLASS  5:CLASS  7:CLASS  8:Atom  9:Atom  10:CLASS
11:CLASS
12:CLASS  13:CLASS  15:CLASS  16:CLASS  17:Atom  18:Atom  19:CLASS  20:CLASS
27:Atom  29:CLASS
32:Atom  33:Atom  34:Atom  35:Atom  36:Atom  37:Atom  41:CLASS  42:Atom  43:Atom
44:Atom  45:CLASS
46:CLASS  47:CLASS  49:Atom  50:CLASS
Element Count :
```

Node 29: Limited
C,C3

L24 96 SEA FILE=MARPAT SSS FUL L1
L25 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation:
Uploading L25.str



chain nodes :
3 4 5 8 9 10 13 14 22 34 38 39 40 43 44 45 46 47 48 49 50 51
52 53 58 59 60 61 63
ring nodes :
1 2 6 7 11 12 21 25 26 27 28 29 30 35 36 37 42
chain bonds :
1-3 1-4 2-5 2-58 6-10 6-59 7-8 7-9 11-14 11-60 12-13 12-61 21-34 21-63
35-39 35-40 37-38 43-44 43-45 43-46 47-48 47-49 47-50 48-51 48-52 48-53
ring bonds :
1-2 6-7 11-12 21-42 21-35 25-26 25-30 26-27 27-28 28-29 29-30 35-36 36-
37
37-42
exact/norm bonds :
1-3 1-4 2-5 2-58 6-10 6-59 7-8 7-9 11-14 11-60 12-13 12-61 21-34 21-63
35-39 35-40 37-38 43-44 43-45 43-46 47-48 47-49 47-50 48-51 48-52 48-53
exact bonds :
1-2 6-7 11-12 21-42 21-35 35-36 36-37 37-42
normalized bonds :
25-26 25-30 26-27 27-28 28-29 29-30

G3:[*1],[*2]

G4:[*3-*4],[*5-*6],[*7-*8]

```
G5:[*9],[*10]

G6:H,[*9]

Connectivity :
22:1 E exact RC ring/chain
Match level :
1:Atom  2:Atom  3:CLASS  4:CLASS  5:CLASS  6:Atom  7:Atom  8:CLASS  9:CLASS
10:CLASS
11:Atom  12:Atom  13:CLASS  14:CLASS  21:Atom  22:Atom  25:Atom  26:Atom  27:Atom
28:Atom  29:Atom
30:Atom  34:CLASS  35:Atom  36:Atom  37:Atom  38:Atom  39:CLASS  40:CLASS  42:Atom
43:Atom
44:CLASS  45:CLASS  46:CLASS  47:Atom  48:Atom  49:CLASS  50:CLASS  51:CLASS
52:CLASS  53:CLASS
58:CLASS  59:CLASS  60:CLASS  61:CLASS  63:CLASS
Element Count :
Node 22: Limited
    C,C3




L27          17 SEA FILE=MARPAT SUB=L24 SSS FUL L25

100.0% PROCESSED      91 ITERATIONS                    17 ANSWERS
SEARCH TIME: 00.00.01



=> s l27 not L48
L54         16 L27 NOT L48

=> dup rem L53 L21 L54
DUPLICATE IS NOT AVAILABLE IN 'BEILSTEIN'.
ANSWERS FROM THESE FILES WILL BE CONSIDERED UNIQUE
FILE 'ZCAPLUS' ENTERED AT 17:00:26 ON 26 MAR 2008
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FILE 'MARPAT' ENTERED AT 17:00:26 ON 26 MAR 2008
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COPYRIGHT (C) 2008 American Chemical Society (ACS)
PROCESSING COMPLETED FOR L53
PROCESSING COMPLETED FOR L21
PROCESSING COMPLETED FOR L54
L55          26 DUP REM L53 L21 L54 (0 DUPLICATES REMOVED)
                ANSWERS '1-6' FROM FILE ZCAPLUS
                ANSWERS '7-10' FROM FILE BEILSTEIN
                ANSWERS '11-26' FROM FILE MARPAT

=> d ibib abs hitind hitstr L55 1-6; d ide allref L55 7-10; d ibib abs qhit L55 11-
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L55 ANSWER 1 OF 26 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2003:777384 ZCAPLUS Full-text
DOCUMENT NUMBER: 139:292150
TITLE: preparation of lactams and lactones as antiinflammatories
INVENTOR(S): Shen, Yaping; Burgoyne, David L.; Lauener, Ronald W.; Zhou, Yuanlin; Rebstein, Patrick J.; Abraham, Samuel D. M.
PATENT ASSIGNEE(S): Inflazyme Pharmaceuticals Ltd., Can.
SOURCE: U.S. Pat. Appl. Publ., 88 pp., Cont.-in-part of U.S. Ser. No. 81,993.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

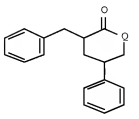
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2003186943	A1	20031002	US 2002-263336	20021001
US 6770658	B2	20040803		
WO 2000014083	A1	20000316	WO 1999-CA819	19990909
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZA, ZW				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
US 6458829	B1	20021001	US 2001-786949	20010511
CA 2500675	A1	20040415	CA 2003-2500675	20030930
WO 2004031149	A1	20040415	WO 2003-CA1506	20030930
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2003271478	A1	20040423	AU 2003-271478	20030930
EP 1551805	A1	20050713	EP 2003-753187	20030930
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
JP 2006508069	T	20060309	JP 2004-540421	20030930
MX 2005PA03547	A	20050701	MX 2005-PA3547	20050401

PRIORITY APPLN. INFO.:		
US 1998-99637P	P	19980909
US 1999-121507P	P	19990223
US 1999-149517P	P	19990817
US 1999-393445	B1	19990908
WO 1999-CA819	W	19990909
US 2000-527699	B1	20000316
US 2001-786949	A2	20010511
US 2002-81993	A2	20020222
US 2002-263336	A	20021001

WO 2003-CA1506 W 20030930

OTHER SOURCE(S): MARPAT 139:292150

GI



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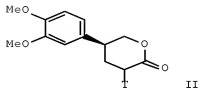


II

AB Title compds., e.g. [I; Q = multivalent atom other than C; each substitutable position may be substituted by W, R7Wn; W = NH2, CONH2, COOH, CN, CHO, OCHO, X, OH, NO2, SH, COX, NHR8, NR8R8, CONHR8, CONR8R8, COOR8, COR8, OCOR8, OR8, BH2, BHR8, BR8R8, BO2H2, BO2R8R8, PH2, PHR8, PR8R8, POR8, PO2R8, PO3R8, SR8; SOR8, SO2R8, SONH2, SONHR8, SONR8R8, SO2NH2, SO2NHR8, SO2NR8R8; R7 = hydrocarbyl, halocarbyl, hydrohalocarbyl wherein n of the H or halo atoms of R7 are substituted by W; R8 = hydrocarbyl, halocarbyl, hydrohalocarbyl; n = 0-5; X = Br, Cl, F, iodo], were prepared Thus, n-BuLi was added to a solution of diisopropylamine in THF at -78 °; the mixture was stirred at -78° for 1 h, then HMPA was added, followed by a solution of (II; T = H) in THF. After 1 h, a solution of 4-(cyclopentyloxy)-3-methoxybenzyl bromide in THF was added to the reaction, and the resulting mixture was stirred at -78° for an addnl. 4 h to give II; T = 4-(cyclopentyloxy)-3-methoxybenzyl. The latter in a murine tail skin allograft transplantation model gave 100% allograft survival at 9 days post-transplant.

IC ICM A61K031-675
ICS A61K031-445; C07D211-40

INCL 514089000; 514317000; 546022000; 546216000

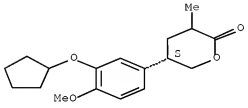
CC 27-16 (Heterocyclic Compounds (One Hetero Atom))
Section cross-reference(s): 1

IT 261357-66-8P 261357-73-7P 261357-79-3P 261357-86-2P 261357-98-6P
261358-04-7P 261358-05-8P 261358-07-0P 261358-09-2P 261358-12-7P
261358-14-9P 261358-15-0P 261358-16-1P 261358-21-8P
261358-22-9P 261358-23-0P 261358-35-4P 261358-40-1P 261358-42-3P
261358-44-5P 261358-46-7P 261358-48-9P 261358-50-3P 261358-51-4P
261358-52-5P 261358-53-6P 261358-54-7P 261358-55-8P 261358-56-9P
261358-58-1P 261358-60-5P 261358-61-6P 261358-62-7P 261358-63-8P
261358-64-9P 261358-65-0P 261358-66-1P 261358-67-2P 261358-68-3P
261358-69-4P 261358-70-7P 261358-71-8P 261358-72-9P 261358-73-0P
261358-74-1P 261358-75-2P 261358-76-3P 261358-77-4P 261358-78-5P
261358-79-6P 261358-80-9P 261358-81-0P 261358-82-1P 261358-83-2P
261358-84-3P 261358-85-4P 261358-86-5P 261358-87-6P 261358-88-7P
261358-89-8P 261358-90-1P 261358-91-2P 261358-92-3P 261358-93-4P
261358-94-5P 261358-95-6P 261358-96-7P 261358-97-8P 261358-98-9P
261358-99-0P 608141-85-1P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of lactams and lactones as antiinflammatories)

IT 261358-15-0P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES

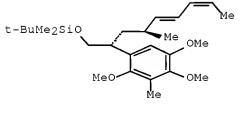
(Uses)
(preparation of lactams and lactones as antiinflammatories)
RN 261358-15-0 ZCAPLUS
CN 2H-Pyran-2-one, 5-[3-(cyclopentyloxy)-4-methoxyphenyl]tetrahydro-3-methyl-, (5S)- (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L55 ANSWER 2 OF 26 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2002:790729 ZCAPLUS Full-text
DOCUMENT NUMBER: 138:24849
TITLE: Synthesis of a Diels-Alder precursor for the Elisabethin A skeleton
AUTHOR(S): Heckrodt, Thilo J.; Mulzer, Johann
CORPORATE SOURCE: Institut fur Organische Chemie der Universitat Wien, Vienna, 1090, Austria
SOURCE: Synthesis (2002), (13), 1857-1866
CODEN: SYNTBF; ISSN: 0039-7881
PUBLISHER: Georg Thieme Verlag
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 138:24849
GI



I

AB A synthesis of a precursor, I, for the elisabethin A skeleton is reported. Containing a masked quinone and a (E,Z)-diene subunit, it has the required elements for the envisaged intramol. Diels-Alder reaction to form the tricyclic system of elisabethin A. Starting from methylresorcinol, the sequence involves the preparation of an arylacetic acid, which was α-alkylated by a chiral building block. Subsequent HWE reaction and cis-selective Wittig olefination furnished the diene with the desired geometry.
CC 30-20 (Terpenes and Terpenoids)

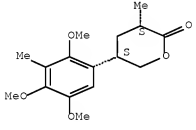
IT 19676-67-6P 212051-35-9P 478303-35-4P 478303-44-5P
478303-53-6P 478303-54-7P 478303-55-8P 478303-61-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of a Diels-Alder precursor for the elisabethin A skeleton from methylresorcinol via α-alkylation of an arylacetic acid by a chiral building block, Horner-Wadsworth Emmons and cis-selective Wittig reactions)

IT 478303-53-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of a Diels-Alder precursor for the elisabethin A skeleton from methylresorcinol via α-alkylation of an arylacetic acid by a chiral building block, Horner-Wadsworth Emmons and cis-selective Wittig reactions)

RN 478303-53-6 ZCAPLUS

CN 2H-Pyran-2-one, tetrahydro-3-methyl-5-(2,4,5-trimethoxy-3-methylphenyl)-, (3S,5S)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



REFERENCE COUNT: 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L55 ANSWER 3 OF 26 ZCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER:	2000:175807 ZCAPLUS Full-text
DOCUMENT NUMBER:	132:222442
TITLE:	Preparation of substituted γ-phenyl-δ-lactones and analogs as antiinflammatory agents
INVENTOR(S):	Shen, Yaping; Burgoyne, David L.; Lauener, Ronald W.; Zhou, Yuanlin; Rebstein, Patrick J.; Abraham, Samuel D. M.
PATENT ASSIGNEE(S):	Inflazyme Pharmaceuticals Ltd., Can.
SOURCE:	PCT Int. Appl., 210 pp. CODEN: PIXXD2
DOCUMENT TYPE:	Patent
LANGUAGE:	English
FAMILY ACC. NUM. COUNT:	2
PATENT INFORMATION:	

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000014083	A1	20000316	WO 1999-CA819	19990909

W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZA, ZW

RW: GH, GM, KE, LS, MW, SD, SL, SZ, UG, ZW, AT, BE, CH, CY, DE, DK,

ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

CA 2343732	A1	20000316	CA 1999-2343732	19990909
AU 9955009	A	20000327	AU 1999-55009	19990909
AU 757052	B2	20030130		
EP 1112262	A1	20010704	EP 1999-941351	19990909
EP 1112262	B1	20040804		

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO

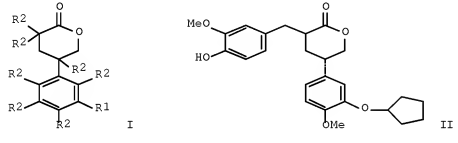
JP 2002524456	T	20020806	JP 2000-568841	19990909
AT 272628	T	20040815	AT 1999-941351	19990909
ES 2226422	T3	20050316	ES 1999-941351	19990909
MX 2001PA02539	A	20021017	MX 2001-PA2539	20010309
US 6458829	B1	20021001	US 2001-786949	20010511
US 2003186943	A1	20031002	US 2002-263336	20021001
US 6770658	B2	20040803		

PRIORITY APPLN. INFO.:

US 1998-99637P	P	19980909
US 1999-121507P	P	19990223
US 1999-149517P	P	19990817
US 1999-393445	B1	19990908
WO 1999-CA819	W	19990909
US 2000-527699	B1	20000316
US 2001-786949	A2	20010511
US 2002-81993	A2	20020222

OTHER SOURCE(S): MARPAT 132:222442

GI



AB The title compds. (I) [wherein R1 = W or R7(W)n; R2 = independently H, W, or R7(W)n; R7 = (halo)carbyl; n = 0-5; W = CONH2, CN, X, NO2, COX, N(R8)2, CO2R8, COR8, OCOR8, OR8, B(R8)2, B(OR8)2, P(R8)2, P(OR8)2, P(O)(OR8)2, SR8, SOR8, SO2R8, SON(R8)2, or SO2N(R8)2; X = halo; R8 = independently H or (halo)carbyl] and their lactams were prepared Examples include syntheses for approx. 90 compds. and data from over 20 bioassays. For instance, II was prepared in a 12-step sequence involving: (1-9) formation of the tert-Bu (S)-5-hydroxy-4-[4-methoxy-3-(pentyloxy)phenyl]pentanoate intermediate starting from 3-hydroxy-4-methoxybenzyl alc., (10) ring closure to give the γ-phenyl-δ-lactone (94%), (11) α-addition of 4-(benzyloxy)-3-methoxybenzyl bromide (70%), and (12) debenzylation of the alc. (83%). II inhibited neutrophil degranulation (IC50 < 1 μM), displayed antioxidant activity against the radical cation ABTS+ (75-100% activity), inhibited resiniferitoxin-induced mouse ear edema (98% by topical administration), and proved effective in reducing the effects of inflammatory bowel disease in rats and in treating existing rheumatoid arthritis in mice. Due to their antiinflammatory and antiproliferative activities, I are useful for the treatment of diseases such as rheumatoid

arthritis, psoriasis, autoimmune disease, inflammatory bowel disease, asthma, graft vs. host disease, and cancer.

IC ICM C07D309-30
ICS C07F005-02; C07D405-10; C07F009-40; C07D211-76; A61K031-35

CC 27-13 (Heterocyclic Compounds (One Hetero Atom))
Section cross-reference(s): 1

IT 261357-66-8P 261357-73-7P 261357-79-3P 261357-86-2P 261357-94-2P
261357-98-6P 261358-05-8P 261358-07-0P 261358-09-2P 261358-12-7P
261358-14-9P 261358-15-0P 261358-16-1P 261358-21-8P
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261358-44-5P 261358-46-7P 261358-48-9P 261358-50-3P 261358-51-4P
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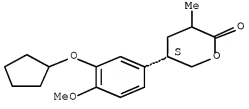
261358-93-4P 261358-94-5P 261358-95-6P 261358-96-7P 261358-97-8P
261358-98-9P 261358-99-0P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(target compound; preparation of substituted γ-phenyl-δ-lactones and lactams as antiinflammatory agents)

IT 261358-15-0P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(target compound; preparation of substituted γ-phenyl-δ-lactones and lactams as antiinflammatory agents)

RN 261358-15-0 ZCAPLUS

CN 2H-Pyran-2-one, 5-[3-(cyclopentyloxy)-4-methoxyphenyl]tetrahydro-3-methyl-, (5S)- (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L55 ANSWER 4 OF 26 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1998:503345 ZCAPLUS Full-text
DOCUMENT NUMBER: 129:230608
TITLE: New Strategies in Carbonylation Chemistry: The Synthesis of δ-Lactones from Saturated Alcohols and CO
AUTHOR(S): Tsunoi, Shinji; Ryu, Ilhyong; Okuda, Tohru; Tanaka, Minoru; Komatsu, Mitsuo; Sonoda, Noboru
CORPORATE SOURCE: Department of Applied Chemistry Faculty of Engineering and Research Center for Environmental Preservation, Osaka University, Osaka, 565-0871, Japan

SOURCE: Journal of the American Chemical Society (1998), 120(34), 8692-8701
CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 129:230608

AB This paper describes the δ-carbonylation of saturated alcs. which uses a 1,5-hydrogen-transfer reaction of alkoxyl radicals and subsequent carbonylation at the δ-carbon atoms as the key. The carbonylation reactions of five classes of saturated alcs., namely, primary alcs. having primary δ-carbons, primary alcs. having secondary δ-carbons, primary alcs. having tertiary δ-carbons, secondary alcs. having primary δ-carbons, secondary alcs. having secondary δ-carbons, were carried out, in which lead tetraacetate (LTA) was used as a one-electron oxidant to generate the alkoxyl radicals. Carbonylation of these saturated alcs., except for primary alcs. having tertiary δ-carbons, took place to afford δ-lactones in moderate to good yields. The mechanism of the remote carbonylation likely involves (1) alkoxyl radical generation via LTA oxidation of a saturated alc., (2) conversion of this alkoxyl radical to a δ-hydroxyalkyl radical by a 1,5-hydrogen-transfer reaction, (3) CO trapping of the δ-hydroxyalkyl radical yielding an acyl radical, and (4) oxidation and cyclization of the acyl radical to give a δ-lactone. A metal salt-free system was also tested for a substrate derived from a tertiary alc. having a secondary δ-carbon; the photolysis of an alkyl 4-nitrobenzenesulfenate under CO pressures gave a δ-lactone in moderate yield.

CC 27-13 (Heterocyclic Compounds (One Hetero Atom))

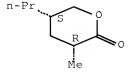
IT 698-76-0P 1004-29-1P 1121-84-2P 14983-21-2P 16429-09-7P
22791-77-1P 24405-13-8P 24405-14-9P 65451-94-7P 65451-95-8P
82390-70-3P 99978-13-9P 142636-30-4P 142636-31-5P 156458-68-3P
156458-70-7P 156458-71-8P 156458-72-9P 156458-73-0P 156458-74-1P
156458-75-2P 156458-76-3P 156458-77-4P 212894-12-7P 212894-13-8P
212894-14-9P 212894-15-0P 212894-16-1P 212894-18-3P
212894-20-7P 212894-22-9P 212894-33-2P 212894-35-4P 212894-40-1P
212894-43-4P 212894-49-0P 212894-52-5P 212894-53-6P
212894-54-7P 212894-55-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of δ-lactones by carbonylation of saturated alcs.)

IT 212894-14-9P 212894-53-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of δ-lactones by carbonylation of saturated alcs.)

RN 212894-14-9 ZCAPLUS

CN 2H-Pyran-2-one, tetrahydro-3-methyl-5-propyl-, (3R,5S)-rel- (CA INDEX NAME)

Relative stereochemistry.

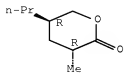


RN 212894-53-6 ZCAPLUS

CN 2H-Pyran-2-one, tetrahydro-3-methyl-5-propyl-, (3R,5R)-rel- (CA INDEX

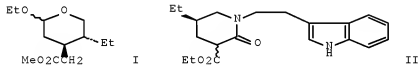
NAME)

Relative stereochemistry.



REFERENCE COUNT: 165 THERE ARE 165 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L55 ANSWER 5 OF 26 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1996:26683 ZCAPLUS Full-text
DOCUMENT NUMBER: 124:146549
TITLE: Synthesis of six-membered compounds by environmentally friendly cyclization using indirect electrolysis
AUTHOR(S): Ihara, Masataka; Katsumata, Akira; Setsu, Fumihito; Tokunaga, Yuji; Fukumoto, Keiichiro
CORPORATE SOURCE: Pharmaceutical Institute, Tohoku University, Aobayama, 980-77, Japan
SOURCE: Journal of Organic Chemistry (1996), 61(2), 677-84
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 124:146549
GI



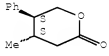
AB [Ni(cyclam)](ClO4)2-catalyzed indirect electroredn. of olefinic bromides produced six-membered compds. in low to high yields. The synthetic intermediate I of Ipecac and Corynanthe alkaloids was obtained in 88% yield in a highly stereoselective manner. Lactam II, the synthetic precursor of tacamonine, was prepared in 49% yield as a mixture of two diastereoisomers. The electrolysis of the bromoacetates gave the debrominated compds. in good yields.

CC 31-5 (Alkaloids)
Section cross-reference(s): 27, 72

IT 94844-37-8P 122937-63-7P 122937-67-1P 155529-27-4P 155529-33-2P 157405-11-3P 163457-30-5P 163457-31-6P 163457-40-7P 163513-91-5P 163513-92-6P 173423-60-4P 173423-61-5P 173423-62-6P 173423-64-8P 173423-65-9P 173423-66-0P 173423-67-1P 173423-70-6P 173423-71-7P 173423-72-8P 173423-78-4P 173423-80-8P 173423-81-9P

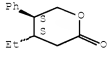
173423-82-0P 173423-83-1P 173423-84-2P 173423-85-3P 173423-86-4P
173423-87-5P 173423-88-6P 173423-89-7P 173423-90-0P 173423-91-1P
173423-93-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(synthesis of six-membered compds. by electrochem. cyclization)
IT 173423-80-8P 173423-81-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(synthesis of six-membered compds. by electrochem. cyclization)
RN 173423-80-8 ZCAPLUS
CN 2H-Pyran-2-one, tetrahydro-4-methyl-5-phenyl-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 173423-81-9 ZCAPLUS
CN 2H-Pyran-2-one, 4-ethyltetrahydro-5-phenyl-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



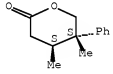
L55 ANSWER 6 OF 26 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1974:520459 ZCAPLUS Full-text
DOCUMENT NUMBER: 81:120459
ORIGINAL REFERENCE NO.: 81:19039a,19042a
TITLE: Epimeric mixtures of the lactone 3,6-dihydro-4,5-dimethyl-5-phenyl-α-pyrone
INVENTOR(S): Van Venrooy, John J.
PATENT ASSIGNEE(S): Sun Research and Development Co.
SOURCE: U.S., 3 pp. Continuation-in-part of U.S. 3,761,530 (CA 79;146293a).
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3825572	A	19740723	US 1972-318359	19721226
US 3761530	A	19730925	US 1972-258282	19720531
PRIORITY APPLN. INFO.:			US 1972-258282 A	19720531

GI For diagram(s), see printed CA Issue.

AB Ph-CHMeCHO was treated with MeCHO and NaOH to give Ph- CHMeCH:C(CHO)CH:CMePh and a mixture of the 2 epimers of the pyranone I.
IC C07D
INCL 260343500
CC 27-13 (Heterocyclic Compounds (One Hetero Atom))
Section cross-reference(s): 25
IT 53655-81-5P 53655-82-6P 53855-97-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
IT 93-53-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with acetaldehyde)
IT 53655-81-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 53655-81-5 ZCAPLUS
CN 2H-Pyran-2-one, tetrahydro-4,5-dimethyl-5-phenyl-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.

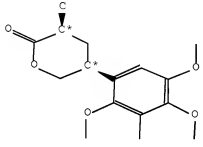


IT 93-53-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with acetaldehyde)
RN 93-53-8 ZCAPLUS
CN Benzeneacetaldehyde, α-methyl- (CA INDEX NAME)

L55 ANSWER 7 OF 26 BEILSTEIN COPYRIGHT 2008 BEILSTEIN MDL on STN

Beilstein Records (BRN):	9208998
Chemical Name (CN):	(3S,5S)-3-methyl-5-(2,4,5-trimethoxy-3-methylphenyl)tetrahydropyran-2-one
Autonom Name (AUN):	3-methyl-5-(2,4,5-trimethoxy-3-methyl-phenyl)-tetrahydro-pyran-2-one
Molec. Formula (MF):	C16 H22 O5
Molecular Weight (MW):	294.35
Lawson Number (LN):	19213, 289
File Segment (FS):	Stereo compound

Compound Type (CTYPE): heterocyclic
Constitution ID (CONSID): 7776828
Tautomer ID (TAUTID): 8646574
Entry Date (DED): 2003/01/18
Update Date (DUPD): 2003/01/18



Field Availability:

Code	Name	Occurrence
BRN	Beilstein Records	1
CN	Chemical Name	1
AUN	Autonomname	1
MF	Molecular Formula	1
FW	Formular Weight	1
LN	Lawson Number	2
FS	File Segment	1
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
ED	Entry Date	1
UPD	Update Date	1
MS	Mass Spectrum	1
NMR	Nuclear Magnetic Resonance	3
ORP	Optical Rotatory Power	1

This substance also occurs in Reaction Documents:

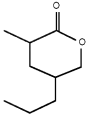
Code	Name	Occurrence
RX	Reaction Documents	1
RXPRO	Substance is Reaction Product	1

All References:
ALLREF

1. Heckrodt, Thilo J.; Mulzer, Johann, Synthesis, CODEN: SYNTBF(13), <2002>, 1857 - 1866; BABS-6363092

L55 ANSWER 8 OF 26 BEILSTEIN COPYRIGHT 2008 BEILSTEIN MDL on STN

Beilstein Records (BRN):	8049582
Chemical Name (CN):	3-methyl-5-propyl-tetrahydro-pyran-2-one
Autonom Name (AUN):	3-methyl-5-propyl-tetrahydro-pyran-2-one
Molec. Formula (MF):	C9 H16 O2
Molecular Weight (MW):	156.22
Lawson Number (LN):	17736
Compound Type (CTYPE):	heterocyclic
Constitution ID (CONSID):	6782509
Tautomer ID (TAUTID):	7529184
Beilstein Citation (BSO):	6-17
Entry Date (DED):	1999/05/06
Update Date (DUPD):	1999/05/07



Field Availability:

Code	Name	Occurrence
BRN	Beilstein Records	1
CN	Chemical Name	1
AUN	Autonomname	1
MF	Molecular Formula	1
FW	Formular Weight	1
LN	Lawson Number	1
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
BSO	Beilstein Citation	1
ED	Entry Date	1
UPD	Update Date	1
IR	Infrared Spectrum	1
NMR	Nuclear Magnetic Resonance	3

This substance also occurs in Reaction Documents:

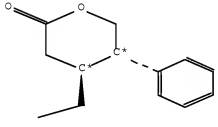
Code	Name	Occurrence
RX	Reaction Documents	1
RXPRO	Substance is Reaction Product	1

All References:
ALLREF

1. Tsunoi, Shinji; Ryu, Ilhyong; Okuda, Tohru; Tanaka, Minoru; Komatsu, Mitsuo; Sonoda, Noboru, J.Amer.Chem.Soc., CODEN: JACSAT, 120(34), <1998>, 8692-8701; BABS-6127724

L55 ANSWER 9 OF 26 BEILSTEIN COPYRIGHT 2008 BEILSTEIN MDL on STN

Beilstein Records (BRN):	7425194
Chemical Name (CN):	(+/-)-(3R*,4R*)-3-ethyl-4-phenyl-5-pentanolide
Autonom Name (AUN):	4-ethyl-5-phenyl-tetrahydro-pyran-2-one
Molec. Formula (MF):	C13 H16 O2
Molecular Weight (MW):	204.27
Lawson Number (LN):	17953
File Segment (FS):	racemate, Stereo compound
Compound Type (CTYPE):	heterocyclic
Constitution ID (CONSID):	6326546
Tautomer ID (TAUTID):	7019664
Beilstein Citation (BSO):	6-17
Entry Date (DED):	1996/08/09
Update Date (DUPD):	1997/04/28



Fragment Notes:
Additionally represents mirror image
Stereo Descriptor: +/-

Field Availability:

Code	Name	Occurrence
BRN	Beilstein Records	1
CN	Chemical Name	1
AUN	Autonomname	1
MF	Molecular Formula	1
FW	Formular Weight	1
LN	Lawson Number	1
FS	File Segment	2
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
BSO	Beilstein Citation	1
ED	Entry Date	1
UPD	Update Date	1
IR	Infrared Spectrum	1

NMR	Nuclear Magnetic Resonance	2

This substance also occurs in Reaction Documents:

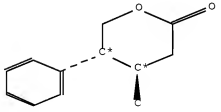
Code	Name	Occurrence
RX	Reaction Documents	1
RXPRO	Substance is Reaction Product	1

All References:
ALLREF

1. Ihara, Masataka; Katsumata, Akira; Setsu, Fumihito; Tokunaga, Yuji; Fukumoto, Keiichiro, J.Org.Chem., CODEN: JOCEAH, 61(2), <1996>, 677-684; BABS-6004130

L55 ANSWER 10 OF 26 BEILSTEIN COPYRIGHT 2008 BEILSTEIN MDL on STN

Beilstein Records (BRN):	7423599
Chemical Name (CN):	(+/-)-(3R*,4R*)-3-methyl-4-phenyl-5-pentanolide
Autonom Name (AUN):	4-methyl-5-phenyl-tetrahydro-pyran-2-one
Molec. Formula (MF):	C12 H14 O2
Molecular Weight (MW):	190.24
Lawson Number (LN):	17944
File Segment (FS):	racemate, Stereo compound
Compound Type (CTYPE):	heterocyclic
Constitution ID (CONSID):	6325158
Tautomer ID (TAUTID):	7015418
Beilstein Citation (BSO):	6-17
Entry Date (DED):	1996/08/09
Update Date (DUPD):	1997/04/28



Fragment Notes:
Additionally represents mirror image
Stereo Descriptor: +/-

Field Availability:

Code	Name	Occurrence
BRN	Beilstein Records	1
CN	Chemical Name	1
AUN	Autonomname	1
MF	Molecular Formula	1

FW	Formular Weight	1
LN	Lawson Number	1
FS	File Segment	2
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
BSO	Beilstein Citation	1
ED	Entry Date	1
UPD	Update Date	1
IR	Infrared Spectrum	1
MP	Melting Point	1
NMR	Nuclear Magnetic Resonance	2

This substance also occurs in Reaction Documents:

Code	Name	Occurrence
RX	Reaction Documents	1
RXPRO	Substance is Reaction Product	1

All References:
ALLREF

1. Ihara, Masataka; Katsumata, Akira; Setsu, Fumihito; Tokunaga, Yuji; Fukumoto, Keiichiro, J.Org.Chem., CODEN: JOCEAH, 61(2), <1996>, 677-684; BABS-6004130

L55 ANSWER 11 OF 26 MARPAT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 146:280341 MARPAT Full-text
TITLE: Hair-styling conditioners containing dicarboxylic acids, organic solvents, and royal jelly, and method of hair modification using them
INVENTOR(S): Ueno, Masako; Kamiyama, Kenichi
PATENT ASSIGNEE(S): Kao Corp., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 15pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2007055918	A	20070308	JP 2005-241664	20050823

PRIORITY APPLN. INFO.: JP 2005-241664 20050823

AB The hair-styling conditioners contain (A) (OH-containing) C≤8 organic dicarboxylic acids or their salts, (B) organic solvents (ClogP -2 to +3) selected from aromatic alcs., N-alkylpyrrolidones, alkylene carbonates, polypropylene glycol, lactones, and cyclic ketones, and (C) royal jelly or its exts. and show pH 2-5 at 25° when diluted 20-fold (by weight) with H2O. The hair conditioners may also contain silicones, oily conditioners, and/or cationic surfactants. A composition (pH 3.7) containing malic acid 5.0, 2-benzyloxyethanol 2.5, glycerin 1.0, EtOH 10.0, royal jelly extract 2.0, NaOH (pH-adjusting agent), and H2O to 100 weight% was applied on human hair and dried, showing hair-styling, -conditioning, and hair elasticity-improving effects. The effects lasted even after shampooing.

G1 = 11

G2 = O
G3 = alkyl (opt. substd. by G4) / Me
G4 = CO2H
Patent location: disclosure
Note: substitution is restricted

L55 ANSWER 12 OF 26 MARPAT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 147:246792 MARPAT Full-text
TITLE: Stripping compositions and method for removing photoresists
INVENTOR(S): Yoon, Seok Il; Kim, Seong Bae; Chung, Jong Hyeon; Park, Hui Jin; Kim, Byeong Uk
PATENT ASSIGNEE(S): Dongjin Semichem Co., Ltd., S. Korea
SOURCE: Faming Zhuanli Shenqing Gongkai Shuomingshu, 18pp. CODEN: CNXXEV
DOCUMENT TYPE: Patent
LANGUAGE: Chinese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
CN 101000467	A	20070718	CN 2007-10000702	20070110
KR 2007074745	A	20070718	KR 2006-2682	20060110
JP 2007188081	A	20070726	JP 2007-2181	20070110

PRIORITY APPLN. INFO.: KR 2006-2682 20060110

AB The compns. for use in lithog. process comprise (un)substituted lactone compds., organic acid or amine compds., and oxidants. The lactone compds. are selected from ≥1 of γ-butyrolactone, γ-methylene γ-butyrolactone, α-methyl-γ-butyrolactone, α-methylene γ-butyrolactone, 2-acetyl butyrolactone, γ-hexalactone, δ-hexalactone, γ-nonalactone, δ-octalactone, γ-valerolactone, and δ-valerolactone. The organic acid compds. are selected from ≥1 of benzoic acid, toluic acid, hydroxybenzoic acid, aminobenzoic acid, citric acid, succinic acid, hydroxy succinic acid, maleic acid, salicylic acid, oxalic acid, phthalic acid, itaconic acid, succinic anhydride, and itaconic anhydride. The organic amines are selected from ≥1 of dimethylethanolamine, diethylmethanolamine, diethylethanolamine, Me diethanolamine, Et dimethanolamine, Et diethanolamine, trimethanolamine, triethanolamine, etc.

The oxidants are selected from ≥1 of H2O2, tert-Bu hydrogen peroxide, benzoyl hydrogen peroxide, etc. The compns. have excellent stripping effect and cause no corrosion to patterned metal films.

MSTP 2

G1 = Me / Pr-n
G2 = 13

Patent location: claim 1

L55 ANSWER 13 OF 26 MARPAT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 146:86862 MARPAT Full-text
TITLE: Hair conditioners containing cationic surfactants or tertiary amines, fatty alcohols, and toluenesulfonates
INVENTOR(S): Tokunaga, Shinichi
PATENT ASSIGNEE(S): Kao Corp., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 15pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2006347997	A	20061228	JP 2005-179589	20050620
US 2007071709	A1	20070329	US 2006-454934	20060619
CN 1891189	A	20070110	CN 2006-10093089	20060620
EP 1754516	A2	20070221	EP 2006-12670	20060620
EP 1754516	A3	20070815		

R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, AL, BA, HR, MK, YU

PRIORITY APPLN. INFO.: JP 2005-179589 20050620

AB The hair conditioners [pH (at 25°) of 20-fold (by weight) aqueous dilution 1-5.5] contain (A) cationic surfactants and/or tertiary amines R1(AR4)aNR2R3 [≥1 of R1-R3 is (are) C8-23 aliphatic hydrocarbyl; the rest of R1-R3 is (are) H, C1-6 alkyl, hydroxyalkyl, benzyl; R4 = C1-6 alkylene; A = CONH, NHCO; a = 0, 1] or their salts, (B) C8-30 fatty alcs., and (C) toluenesulfonic acid or its salts. The hair conditioners may also contain specific organic solvents. An

aqueous hair conditioner composition (pH 3.5) containing stearyltrimethylammonium chloride 1.5, stearyl alc. 3, behenyl alc. 3, p-toluenesulfonic acid 0.1 weight%, etc., was effective for recovery of hair damaged by bleaching.

NSTR 3

G1 = O
G2 = alkyl (substd. by CO2H) / Me
G3 = (1-3) 12

Patent location: claim 2
Note: substitution is restricted

L55 ANSWER 14 OF 26 MARPAT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 145:425245 MARPAT Full-text
TITLE: Conditioning shampoos containing amino-modified silicones and hydrophobic sulfonic acids
INVENTOR(S): Tokunaga, Shinichi
PATENT ASSIGNEE(S): Kao Corp., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 18pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2006282615	A	20061019	JP 2005-106452	20050401

PRIORITY APPLN. INFO.: JP 2005-106452 20050401

AB This invention relates to shampoos for damaged hair which provide excellent foamability, rinsability, and textures in high humidity. The shampoos (pH 2-6) comprise (1) amino-modified silicones, (2) hydrophobic sulfonic acids or salts thereof, (3) hydroxycarboxylic acids, dicarboxylic acids, and/or aromatic carboxylic acids, and (4) organic solvents. For example, a shampoo (pH 3.7) contained amino-modified silicone (Conditioning agent 8500) 0.3, p-toluenesulfonic acid 0.5, malic acid 0.5, lactic acid 0.2, ethanol 0.5, benzyl alc. 0.5, polypropylene glycol 0.3, PEG lauryl ether sulfate Na salt 12, amidopropylbetaine 2, PEG lauryl ether 1, cationic hydroxyethyl cellulose 0.5, Merquat 550 0.2, Silicone CF2450 2, KT1989 0.3, myristyl alc. 0.5, NaOH 0.2, and distilled water balance to 100 %.

NSTR 2

G1 = O
G2 = alkyl (substd. by CO2H) / Me
G3 = (1-3) 12

Patent location: claim 1
Note: substitution is restricted

L55 ANSWER 15 OF 26 MARPAT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 145:425244 MARPAT Full-text
TITLE: Shampoos containing hydrophobic sulfonic acids
INVENTOR(S): Tokunaga, Shinichi
PATENT ASSIGNEE(S): Kao Corp., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 16pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2006282613	A	20061019	JP 2005-106450	20050401

PRIORITY APPLN. INFO.: JP 2005-106450 20050401

AB This invention relates to shampoos for damaged hair which provide excellent dry hair combability. The shampoos (pH 2-6) comprise (1) monoalkyl glyceryl ethers or monoalkenyl glyceryl ethers, (2) hydrophobic sulfonic acids or salts thereof, (3) hydroxycarboxylic acids, dicarboxylic acids, and/or aromatic carboxylic acids, and (4) organic solvents. For example, a shampoo (pH 3.7) contained isodecyl glyceryl ether 1, p-toluenesulfonic acid 0.5, malic acid 0.5, lactic acid 0.2, ethanol 0.5, benzyl alc. 0.5, polypropylene glycol 0.3, PEG lauryl ether sulfate Na salt 12, amidopropylbetaine 2, PEG lauryl ether 1, cationic hydroxyethyl cellulose 0.5, Merquat 550 0.2, Silicone CF2450 2, KT1989 0.3, myristyl alc. 0.5, NaOH 0.2, and distilled water balance to 100 %.

MSTR 2

G1 = O
G2 = alkyl (substd. by CO2H) / Me
G3 = (1-3) 12

Patent location: claim 1
Note: substitution is restricted

L55 ANSWER 16 OF 26 MARPAT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 145:382947 MARPAT Full-text
TITLE: Hair cleansing composition comprising a sulfate surfactant, a sulfonate, and a carboxylate
INVENTOR(S): Tokunaga, Shinichi
PATENT ASSIGNEE(S): Kao Corporation, Japan
SOURCE: Eur. Pat. Appl., 21 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 1707239	A2	20061004	EP 2006-6960	20060331
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK, BA, HR, IS, YU				
JP 2006282614	A	20061019	JP 2005-106451	20050401
CN 1853600	A	20061101	CN 2006-10066912	20060330
US 2006223728	A1	20061005	US 2006-393921	20060331

PRIORITY APPLN. INFO.: JP 2005-106451 20050401

AB The invention relates to a hair cleansing composition comprising (A) a sulfate surfactant, (B) a C6-18 hydrophobic sulfonic acid or salt thereof, (C) a hydroxycarboxylic acid, dicarboxylic acid or aromatic carboxylic acid, and (D) an organic solvent; and having a pH of 2 to 6. A sulfate surfactant, represented by the formula R1-O-(C2H4O)n-SO3M (R1 = C10-18 alkyl or alkenyl; n = 0 or a pos. integer; M = ammonium, Na) is composed of 30 to 45 weight% of a sulfate exhibiting n = 0, 18 to 27 weight% of a sulfate exhibiting n = 1, 10 to 20 weight% of a sulfate exhibiting n = 2, and the balance of sulfates exhibiting n = 3 or greater, and containing the sulfates exhibiting n = 0 to 2 in a total amount of 70 weight% or greater based on the total sulfates,. The hair cleansing composition according to the present invention is excellent in the hair feel during shampooing and effects for straightening the flyaway or waved hair tip, which has resulted from the accumulation of damages caused, for example, by hair coloring. Thus, a hair cleansing composition was prepared containing ammonium lauryl ether sulfate with an average of 1.0 mol of EO (preparation given) 48, p-toluenesulfonic acid 0.5, malic acid 0.5, ethanol 0.5, benzyl alc. 0.5, polypropylene glycol 0.3, amidopropylbetaine 2, cocoylmonoethanolamide 1, polyoxyethylene lauryl ether 0.8, cationic hydroxyethyl cellulose 0.5, Merquat 550 0.2, Silicone CF2450 2, amino-modified silicone KT1989 0.3, myristyl alc. 0.5, ethylene glycol distearate 2, KOH as needed for pH 3.7, and water to 100 weight%, resp.

MSTR 4

G1 = O
G2 = alkyl (substd. by CO2H) / Me
Patent location: claim 1
Note: substitution is restricted

L55 ANSWER 17 OF 26 MARPAT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 143:45571 MARPAT Full-text
TITLE: Compositions containing lactone compatibilizers
INVENTOR(S): Fagan, Paul Joseph; Minor, Barbara Haviland; Shuey, Steven W.; Mahler, Walter
PATENT ASSIGNEE(S): USA
SOURCE: U.S. Pat. Appl. Publ., 24 pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2005127321	A1	20050616	US 2004-965322	20041014

PRIORITY APPLN. INFO.: US 2003-511881P 20031015

AB The present invention relates to compns. that are useful for compatibilizing a conventional compression refrigeration lubricant and a hydrofluorocarbon and/or hydrochlorofluorocarbon refrigerant in a compression refrigeration or air conditioning system. Addnl., these compns. promote efficient return of lubricant from the non-compressor zones to the compressor zones of refrigeration and air conditioning systems.

MSTR 1

G1 = Pr-n
G2 = 16

G3 = Me
Patent location: claim 1

L55 ANSWER 18 OF 26 MARPAT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 140:222914 MARPAT Full-text
TITLE: Storage-stable acidic conditioning shampoo compositions with good foamability for imparting gloss, smoothness, and wet feel to hair
INVENTOR(S): Terasaki, Hiroyuki
PATENT ASSIGNEE(S): Kao Corp., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 15 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2004075545	A	20040311	JP 2002-233706	20020809
JP 3843051	B2	20061108		
PRIORITY APPLN. INFO.:			JP 2002-233706	20020809

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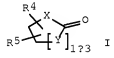

AB Title compns. contain (A) dicarboxylic acids, hydroxycarboxylic acids, or their salts, (B) organic solvents chosen from R1(OCH2CH2)p[OCH2CH((CH2)rY)]qZ [R1 = H, lower alkyl, 4-R2C6H4R3; R2 = H, Me, MeO; R3 = bond, C1-3 (un)saturated divalent hydrocarbylene; Y, Z = H, OH; p, q, r = 0-5; when p = q = 0, then Z ≠ H and R1 = alkyl], N-C1-18 alkylpyrrolidone, C1-4 alkylene carbonates, polypropylene glycol with mo. weight 200-5000, and lactones or cyclic ketones I (X = CH2, O; R4, R5 = substituent; R4 ≠ R5; a, b = 0, 1; s = 1-3), (C) sulfate-type anionic surfactants, and (D) vitamins, amino acids, amino acid analogs, protein hydrolyzates, or their derivs., and show pH 1-4 at 25° when 20-fold diluted in water. Thus, a shampoo (pH 3.5 when 20-fold diluted in water) containing malic acid, benzyloxyethanol, polyoxyethylene lauryl ether sulfate Na salt, Na lauryl sulfate, panthenol, and pantothenyl Et ether showed good hair treatment effect and no change when stored at 50° for 1 mo.

NSTR 1

G1═O

G1 = 30

G5 = alkyl (substd. by G8) / Me
G8 = CO2H
Patent location: claim 1
Note: substitution is restricted

L55 ANSWER 19 OF 26 MARPAT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 140:222871 MARPAT Full-text
TITLE: Storage-stable acidic conditioning shampoo compositions with good foamability for imparting gloss and softness to hair
INVENTOR(S): Terasaki, Hiroyuki
PATENT ASSIGNEE(S): Kao Corp., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 13 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2004075544	A	20040311	JP 2002-233705	20020809
JP 3964759	B2	20070822		

PRIORITY APPLN. INFO.: JP 2002-233705 20020809

AB Title compns. contain sulfate-type anionic surfactants, cationic polymers, and inorg. acids or their salts, and show pH 1-4 at 25° when 20-fold diluted in water. Thus, a shampoo (pH 3.5 when 20-fold diluted in water) containing polyoxyethylene lauryl ether sulfate Na salt, Na lauryl sulfate, cationized cellulose, cationized guar gum, and HCl showed good hair treatment effect and no change when stored at 50° for 1 mo.

MSTR 1

G1═O

G1 = 30

G5 = alkyl (substd. by G8) / Me
G8 = CO2H
Patent location: claim 1
Note: substitution is restricted

L55 ANSWER 20 OF 26 MARPAT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 136:279325 MARPAT Full-text
TITLE: Preparation and use of amido-lactone integrin antagonists
INVENTOR(S): Ruminiski, Peter; Penning, Thomas D.; Jiang, Lan; Balekudru, Devadas; Rogers, Thomas; Yuan, Chester; Vancamp, Jennifer
PATENT ASSIGNEE(S): Pharmacia Corporation, USA
SOURCE: PCT Int. Appl., 88 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002026227	A1	20020404	WO 2001-US30194	20010927
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 2002045645	A1	20020418	US 2001-963926	20010926
US 6720327	B2	20040413		
CA 2423434	A1	20020404	CA 2001-2423434	20010927
AU 2001094776	A5	20020408	AU 2001-94776	20010927
EP 1320363	A1	20030625	EP 2001-975450	20010927
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
JP 2004513088	T	20040430	JP 2002-530057	20010927
US 2004019206	A1	20040129	US 2003-381831	20030327
US 2004116472	A1	20040617	US 2003-717238	20031119
US 6906051	B2	20050614		
PRIORITY APPLN. INFO.:			US 2000-235617P	20000927
			US 2000-241633P	20001010
			US 2001-963926	20001010
			WO 2001-US30194	20010927

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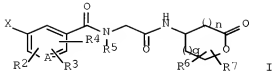

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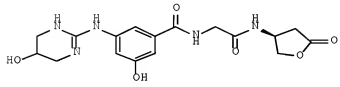
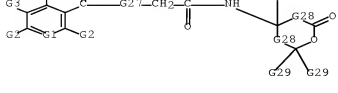


II

AB Title compds. I [X = NHC:YNR8R9, NHC:NR1NR8R9, etc.; Y = NR1, O, S: p, q = 0-3; A = N, C; R1 = H, alkyl, aryl, hydroxy, alkoxy, cyano, nitro, amino, alkenyl, alkynyl, amido, etc. or R1 taken together with R8 forms a 4-12 membered heterocycle; R8 (when not taken together with R1), R9 = H, alk(en/yn)yl, aralkyl, amino, alkylamino, hydroxy, alkoxy, arylamino, amido, alkylcarbonyl, arylcarbonyl, alkoxycarbonyl, aryloxy, aryloxycarbonyl, haloalkylcarbonyl, haloalkoxycarbonyl, alkylthiocarbonyl, arylthiocarbonyl, acyloxymethoxycarbonyl, etc. or NR8 and R9 taken together form a 4-12 membered heterocycle; R2-4 = H, alkyl, hydroxy, alkoxy, aryloxy, halogen, haloalkyl, haloalkoxy, nitro, amino, alkylamino, acylamino, dialkylamino, cyano, alkylthio, etc.; R5-7 = H, alk(en/yn)yl, aryl, carboxy derivs., haloalkyl, cycloalkyl, monocyclic heterocycles, monocyclic heterocycles optionally substituted with alkyl, halogen, haloalkyl, cyano, hydroxy, aryl, fused aryl, nitro, alkoxy, aryloxy, alkylsulfonyl, arylsulfonyl, sulfonamide, thio, alkylthio, carboxy derivs., amino, amido, etc.] were prepared For instance, (4S)-4-aminodihydro-2(3H)furanone hydrochloride (preparation given) was reacted with Boc-Gly-OSu (DMF, NMM, 0°C, 18 h) and the product deprotected with 4N HCl. The intermediate amine was condensed with the corresponding carboxylic acid (prior art, DMF, CH2Cl2, DCC, NMM, 18 h) to give II isolated as the TFA salt. Example compds. had IC50 = 0.1 nM - 100 nM for the αvβ3 integrin and IC50 < 50μM for the αvβ5 integrin. I are useful for the treatment of tumor metastasis, solid tumor growth, macular degeneration, etc.

MSTP 1



G28 = (0-3) 112

G29 = alkyl <containing 1-10 C> (substd. by CO2H) / Me
Patent location: claim 1
Note: and tautomers and polymorphs
Stereochemistry: and isomers, enantiomers and racemates

REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L55 ANSWER 21 OF 26 MARPAT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 138:14020 MARPAT Full-text
TITLE: Preparation of a lactam aldehyde compound
INVENTOR(S): Izumi, Hiroshi; Futamura, Shigeru
PATENT ASSIGNEE(S): Director-General of National Institute of Advanced Industrial Science and Technology, Japan
SOURCE: Eur. Pat. Appl., 10 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 1262479	A1	20021204	EP 2002-251706	20020311
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
JP 2002356476	A	20021213	JP 2001-159742	20010528
JP 3774763	B2	20060517		
US 2002198386	A1	20021226	US 2002-91459	20020307
US 6639075	B2	20031028		
PRIORITY APPLN. INFO.:			JP 2001-159742	20010528

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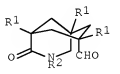

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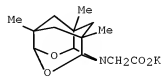
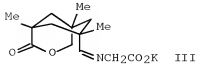


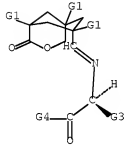
II



III

AB A lactam aldehyde I [R1 = alkyl; R2 = CHR3COR4; R3 = H, amino acid side chain; R4 = OH, peptide side chain, salt of OH] were prepared for use as mol. recognition agents in neurotransmission studies, intermediates for protein analogs, surfactants, protective groups, or hosts for host-guest complexes (no data). Thus, the dioxaazawurtzitane II was rearranged to the lactone imine III by treatment with aqueous MeCN at room temperature for 3 days. III was then stirred in Me2SO at room temperature for 5 days to give I [R1 = Me, R2 = CH2CO2H].

MSTR 2



G1 = Me / Pr-n
Patent location: claim 5

REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

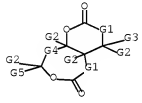
L55 ANSWER 22 OF 26 MARPAT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 132:278654 MARPAT Full-text
TITLE: Emulsifiers for fertilizer emulsion compositions
INVENTOR(S): Bush, James H.
PATENT ASSIGNEE(S): Lubrizol Corp., USA
SOURCE: U.S., 17 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 6054493	A	20000425	US 1998-222662	19981230
CA 2357040	A1	20000713	CA 1999-2357040	19991215
WO 2000040327	A1	20000713	WO 1999-US29686	19991215
W: AU, CA				
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
EP 1140346	A1	20011010	EP 1999-965261	19991215
EP 1140346	B1	20040317		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
AU 769406	B2	20040129	AU 2000-31214	19991215

PRIORITY APPLN. INFO.: US 1998-222662 19981230
WO 1999-US29686 19991215

AB Nonexplosive fertilizer emulsion compns. comprise an aqueous phase (e.g., containing NH4NO3, Zn(NO3)2, urea), an organic phase, and an emulsifier composition comprising the reaction product of an amine having ≥1 NH group and an intermediate formed in the reaction of ≥1 olefinic compound (e.g., polyisobutene) containing ≥1 C=CCH group and ≥1 carboxylic reactant (e.g., glyoxylic acid) selected from compds. of formula R3C(O)(R4)nC(O)OR5 where R3,R5 are sep. H, hydrocarbyl; R4 is a divalent hydrocarbyl group; n is 0 or 1; and ≥1 aldehyde (e.g, formaldehyde) or ketone.

MSTR 4



G1 = bond
G2 = Me
G4 = CH2 (opt. substd. by G7)
G7 = Pr-n
Patent location: claim 23

REFERENCE COUNT: 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L55 ANSWER 23 OF 26 MARPAT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 132:207762 MARPAT Full-text
TITLE: Preparation of pyranones
INVENTOR(S): Abe, Nobuki
PATENT ASSIGNEE(S): Nippon Zeon Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 8 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2000080090	A	20000321	JP 1998-247563	19980901

PRIORITY APPLN. INFO.: JP 1998-183787 19980630
OTHER SOURCE(S): CASREACT 132:207762
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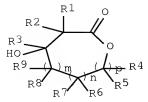

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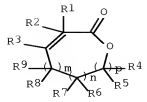

II

AB Title compds. I (R1-R2, R4-R9 = H, NO2, cyano, C1-6 alkyl, alkenyl, aryl; R3 = H, C1-6 alkyl, alkenyl, aryl; m, n, p = 0-1; m = n = p ≠ 0) or II (R2, R4-R9, R3, m, n, p = same as I) are prepared by cyclization of XCR1R2CO2(CR4R5)r(CR6R7)s(CR8R9)tCOR3 (X = halo; R1-R9, m, n, p = same as I) in the presence of transition metals. 3-Oxobutyl bromoacetate (preparation given) was cyclized in the presence of Zn and I in C6H6 under heating for 80 min to give 76% mevalonolactone.

MSTR 2

G1 = Pr-n
G2 = 15

G3 = Me
Patent location: claim 1

L55 ANSWER 24 OF 26 MARPAT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 117:212305 MARPAT Full-text
TITLE: Process for the preparation of α-alkyl lactones, useful as aroma chemicals, from α-acyl lactones
INVENTOR(S): Rebrovic, Louis; Harris, Eugene G.
PATENT ASSIGNEE(S): Henkel K.-G.a.A., USA
SOURCE: PCT Int. Appl., 48 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9209590	A1	19920611	WO 1991-US8745	19911125
W: JP				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LU, NL, SE				
DE 4027241	A1	19910307	DE 1990-4027241	19900829
GB 2235451	A	19910306	GB 1990-19012	19900831
FR 2651496	A1	19910308	FR 1990-10899	19900831
NL 9001922	A	19910402	NL 1990-1922	19900831
JP 03130276	A	19910604	JP 1990-232287	19900831
US 5231192	A	19930727	US 1990-619797	19901129
EP 559789	A1	19930915	EP 1992-901529	19911125
R: BE, DE, FR, GB, IT, NL				
JP 06503328	T	19940414	JP 1992-501551	19911125

PRIORITY APPLN. INFO.: US 1990-619797 19901129
US 1989-315109 19890224
US 1989-402105 19890901
WO 1991-US8745 19911125

OTHER SOURCE(S): CASREACT 117:212305

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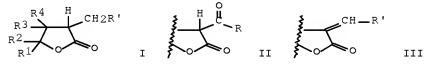
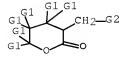


AB α-Alkyl-γ-butyrolactones I (R1-R4, R' = H, C1-20 hydrocarbyl), useful in fragrances, are prepared in 2 steps: (A) reaction of acyl lactones II (R = C1-8 alkyl) with aldehydes R'CHO and alkali metal hydroxides at 50-150° in an inert diluent while removing H2O of reaction, and (B) selective hydrogenation of the formed alkylidene lactones III. Similar preparation of α-alkyl-δ-valerolactones is also claimed. For example, II (R = R1 = Me; R2-R4 = H) (prepared from Et acetoacetate and propylene oxide) was refluxed with heptaldehyde and NaOH under Dean-Stark conditions in PhMe to give 54.5% III [R' = (CH2)5Me; R1-R4 as given], which was hydrogenated over 5% Pd/C in EtOH to give 95% cis-I [R1 = Me; R2-R4 = H; R' = (CH2)5Me]. The latter, a preferred I, has a nutty, pecan odor.

MSTR 4



G1 = Ph (opt. substd. by alkyl <containing 1-8 C>)
Patent location: claim 13

L55 ANSWER 25 OF 26 MARPAT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 118:59572 MARPAT Full-text
TITLE: Preparation of lactones
INVENTOR(S): Abe, Yutaka; Imoto, Hiroyuki; Sotodani, Koshiro
PATENT ASSIGNEE(S): Kao Corp., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 4 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 04261167	A	19920917	JP 1991-20708	19910214
JP 3021700	B2	20000315		
PRIORITY APPLN. INFO.:			JP 1991-20708	19910214

OTHER SOURCE(S): CASREACT 118:59572

AB Lactones are prepared by dehydrocyclization of compds. having ≥2 OH, in which 2 OH are combines with (un)substituted 4-6 carbons, and one of the 2 OH is primary OH, in the presence of catalysts containing Cu, transition metals of 4th period and Pt-group elements. A mixture of 1,4-butanediol and a catalyst [prepared from Cu nitrate, Zn(NO3)2, and RuCl3] was bubbled with H at 190° for 5 h to give 97% γ-butyrolactone.

MSTR 2

G1 = (2-4) 6

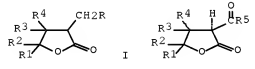
G2 = Me / CH2CH=CH2
Patent location: disclosure

L55 ANSWER 26 OF 26 MARPAT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 114:101715 MARPAT Full-text
TITLE: Preparation of α-alkyl lactones
INVENTOR(S): Rebrovic, Louis; Harris, Eugene G.
PATENT ASSIGNEE(S): Henkel Corp., USA
SOURCE: Ger. Offen., 10 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent

LANGUAGE: German
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 4005515	A1	19900830	DE 1990-4005515	19900222
US 4980342	A	19901225	US 1989-402105	19890901
GB 2228481	A	19900829	GB 1990-4142	19900223
GB 2228481	B	19920415		
NL 9000443	A	19900917	NL 1990-443	19900223
JP 02273667	A	19901108	JP 1990-44309	19900223
BE 1003310	A5	19920225	BE 1990-200	19900223
FR 2643635	A1	19900831	FR 1990-2350	19900226
DE 4027241	A1	19910307	DE 1990-4027241	19900829
GB 2235451	A	19910306	GB 1990-19012	19900831
FR 2651496	A1	19910308	FR 1990-10899	19900831
NL 9001922	A	19910402	NL 1990-1922	19900831
JP 03130276	A	19910604	JP 1990-232287	19900831
PRIORITY APPLN. INFO.:			US 1989-315109	19890224
			US 1989-402105	19890901

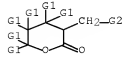
GI



I II

AB α-Alkyl butyrolactones I [R1, R2, R3, R4 = C1-8 alkyl, C3-6 cycloalkyl, (C1-8 alkyl)phenyl, (C1-8 alkyl)benzyl; R = H, C1-8 alkyl or alkenyl, C3-8 cycloalkyl or cycloalkenyl, (substituted) Ph or benzyl] and corresponding valerolactones were prepared by condensation of, e.g., α-acyl butyrolactones II (R5 = C1-8 alkyl) with RCHO in the presence of an alkali metal hydroxide, followed by catalytic hydrogenation. E.g., reaction of 3-acetyl-5-methyldihydro-2(3H)-furanone (III) with cyclohexanecarboxaldehyde in the presence of NaOH in refluxing PhCH3, followed by hydrogenation using 5% Pt-C catalyst gave title compound I (R = cyclohexyl, R1 = Me, R2, R3, R4 = H) in 50% yield. III was prepared by alkylation and intramol. cyclization of Et acetoacetate with propylene oxide.

MSTR 4



G1 = Ph (opt. substd. by 1 or more alkyl <containing 1-8 C>)

Patent location: claim 12

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=>  d his full

     (FILE 'HOME' ENTERED AT 16:29:09 ON 26 MAR 2008)

     FILE 'REGISTRY' ENTERED AT 16:29:23 ON 26 MAR 2008
L1                STRUCTURE UPLOADED
L2                STRUCTURE UPLOADED
L3             0 SEA SSS SAM L1 AND L2
L4             0 SEA SSS SAM L1

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L5             1 SEA ABB=ON  PLU=ON  US2005-529290   /AP
                D SCA
                SEL RN

     FILE 'REGISTRY' ENTERED AT 16:31:30 ON 26 MAR 2008
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                BI OR 13284-42-9/BI OR 1530-32-1/BI OR 23727-15-3/BI OR
                28219-60-5/BI OR 28219-61-6/BI OR 609-02-9/BI OR 623-36-9/BI
                OR 65113-99-7/BI OR 677326-31-7/BI OR 677326-32-8/BI OR
                677326-33-9/BI OR 677326-34-0/BI OR 677326-35-1/BI OR 677326-36
                -2/BI OR 677326-37-3/BI OR 677326-38-4/BI OR 677326-39-5/BI OR
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                -1/BI OR 677326-44-2/BI OR 677326-45-3/BI OR 677326-46-4/BI OR
                677763-76-7/BI OR 677763-77-8/BI OR 67801-20-1/BI OR 72089-08-8
                /BI OR 93-53-8/BI)
L7            14 SEA ABB=ON  PLU=ON  L6 AND OC5/ES
                D SCA
                D RN 1
L8                STR 677763-77-8
                D L8
                D STAT QUE L4
L9            16 SEA SSS FUL L1
                SAVE TEMP L9 CHA290STR1L/A
L10            9 SEA ABB=ON  PLU=ON  L9 AND L7
L11            5 SEA ABB=ON  PLU=ON  L7 NOT L10
                D SCA
L12         6097 SEA ABB=ON  PLU=ON  C10H18O2/MF
L13            1 SEA ABB=ON  PLU=ON  L11 AND L12

     FILE 'ZCAPLUS' ENTERED AT 16:35:26 ON 26 MAR 2008
L14            7 SEA ABB=ON  PLU=ON  L9
L15            1 SEA ABB=ON  PLU=ON  L13 AND L14
L16            2 SEA ABB=ON  PLU=ON  L6 AND L14
                D SCA

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L17            0 SEA SSS SAM L1
L18            0 SEA SSS SAM L1 AND L2
L19              SCREEN 1338
L20            0 SEA SSS SAM L1 AND L19
L21            4 SEA SSS FUL L1 AND L19
L22            4 SEA ABB=ON  PLU=ON  L21/COM

     FILE 'MARPAT' ENTERED AT 16:43:26 ON 26 MAR 2008
L23            5 SEA SSS SAM L1
L24           96 SEA SSS FUL L1
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L25             STRUCTURE UPLOADED
L26           0 SEA SUB=L24 SSS SAM L25
L27          17 SEA SUB=L24 SSS FUL L25
L28         112 SEA ABB=ON  PLU=ON  COSME?/BI
L29         112 SEA ABB=ON  PLU=ON  COSME?/BI,IT
L30           0 SEA ABB=ON  PLU=ON  L24 AND L28

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L31       89969 SEA ABB=ON  PLU=ON  COSME?/BI
L32       36798 SEA ABB=ON  PLU=ON  ?PERFUM?/BI
L33           1 SEA ABB=ON  PLU=ON  L9 (L) COS/RL
L34           1 SEA ABB=ON  PLU=ON  L14 AND (L31 OR L32)
L35       17804 SEA ABB=ON  PLU=ON  TANAKA S?/AU
L36        5183 SEA ABB=ON  PLU=ON  FUKUDA K?/AU
L37         998 SEA ABB=ON  PLU=ON  ASADA T?/AU
L38           1 SEA ABB=ON  PLU=ON  L35 AND L36 AND L37
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L40           1 SEA ABB=ON  PLU=ON  L36 AND L37
L41          85 SEA ABB=ON  PLU=ON  (L35 OR L36 OR L37) AND L32
L42           1 SEA ABB=ON  PLU=ON  L38 OR L40
L43          11 SEA ABB=ON  PLU=ON  L39 AND L32

     FILE 'HCAPLUS' ENTERED AT 16:55:21 ON 26 MAR 2008
L44          17 SEA ABB=ON  PLU=ON  L27
L45          96 SEA ABB=ON  PLU=ON  L24
L46           1 SEA ABB=ON  PLU=ON  L45 AND (L35 OR L36 OR L37)
                SEL AN

     FILE 'MARPAT' ENTERED AT 16:55:57 ON 26 MAR 2008
L47           1 SEA ABB=ON  PLU=ON  ("140:321236"/AN OR "2004:292019"/AN)
L48           1 SEA ABB=ON  PLU=ON  L47 AND L27

     FILE 'REGISTRY' ENTERED AT 16:56:29 ON 26 MAR 2008

     FILE 'ZCAPLUS' ENTERED AT 16:56:32 ON 26 MAR 2008
               D STAT QUE L38
               D STAT QUE L43

     FILE 'WPIX' ENTERED AT 16:56:54 ON 26 MAR 2008
L49          10 SEA ABB=ON  PLU=ON  L39 AND L32

     FILE 'STNGUIDE' ENTERED AT 16:57:04 ON 26 MAR 2008

     FILE 'ZCAPLUS, WPIX' ENTERED AT 16:57:13 ON 26 MAR 2008
L50          41 DUP REM L38 L39 L49 (11 DUPLICATES REMOVED)
                    ANSWERS '1-41' FROM FILE ZCAPLUS
L51          11 DUP REM L38 L43 L49 (11 DUPLICATES REMOVED)
                    ANSWERS '1-11' FROM FILE ZCAPLUS
               D IBIB ABS HITIND HITSTR L51 1-11

     FILE 'MARPAT' ENTERED AT 16:58:25 ON 26 MAR 2008
               D STAT QUE L48
               D IBIB ABS QHIT 1 L48

     FILE 'REGISTRY' ENTERED AT 16:58:53 ON 26 MAR 2008

     FILE 'ZCAPLUS' ENTERED AT 16:58:56 ON 26 MAR 2008
               D STAT QUE L14
               D STAT QUE L15
               D STAT QUE L16
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                D STAT QUE L33
                D STAT QUE L34
L52           7 SEA ABB=ON  PLU=ON  (L14 OR L15 OR L16) OR (L33 OR L34)
L53           6 SEA ABB=ON  PLU=ON  L52 NOT (L38 OR L43)

     FILE 'BEILSTEIN' ENTERED AT 16:59:48 ON 26 MAR 2008
                D STAT QUE L21

     FILE 'MARPAT' ENTERED AT 17:00:01 ON 26 MAR 2008
                D STAT QUE L27
L54          16 SEA ABB=ON  PLU=ON  L27 NOT L48

     FILE 'ZCAPLUS, BEILSTEIN, MARPAT' ENTERED AT 17:00:26 ON 26 MAR 2008
L55          26 DUP REM L53 L21 L54 (0 DUPLICATES REMOVED)
                    ANSWERS '1-6' FROM FILE ZCAPLUS
                    ANSWERS '7-10' FROM FILE BEILSTEIN
                    ANSWERS '11-26' FROM FILE MARPAT
                D IBIB ABS HITIND HITSTR L55 1-6
                D IDE ALLREF L55 7-10
                D IBIB ABS QHIT L55 11-26


     FILE HOME

     FILE REGISTRY
     Property values tagged with IC are from the ZIC/VINITI data file
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     STRUCTURE FILE UPDATES:   25 MAR 2008  HIGHEST RN 1010115-69-1
     DICTIONARY FILE UPDATES:  25 MAR 2008  HIGHEST RN 1010115-69-1

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     FILE ZCAPLUS

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     FILE COVERS 1907 - 26 Mar 2008  VOL 148 ISS 13
     FILE LAST UPDATED: 25 Mar 2008  (20080325/ED)
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FILE BEILSTEIN
FILE LAST UPDATED ON January 3, 2008

FILE COVERS 1771 TO 2007.
 FILE CONTAINS 10,119,480  SUBSTANCES

>>>PLEASE NOTE: Reaction Data and substance data are stored in
   separate documents and can not be searched together in one query.
   Reaction data for BEILSTEIN compounds may be displayed
   immediately with the display codes PRE (preparations) and REA
   (reactions).  A substance answer set retrieved after the search
   for a chemical name, a compounds with available reaction
   information by combining with PRE/FA, REA/FA or more generally
   with RX/FA. The BEILSTEIN Registry Number (BRN) is the link
   between a BEILSTEIN compound and belonging reactions. For mo
   detailed reaction searches BRNs can be searched as reaction
   partner BRNs Reactant BRN (RX.RBRN) or Product BRN (RX.PBRN).<<<

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>>> Price change as of January 1st, 2008: Connect Time and Structure
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FILE MARPAT
FILE CONTENT: 1961-PRESENT VOL 148 ISS 11 (20080321/ED)

SOME MARPAT RECORDS ARE DERIVED FROM INPI DATA FOR 1961-1987

MOST RECENT CITATIONS FOR PATENTS FROM MAJOR ISSUING AGENCIES
(COVERAGE TO THESE DATES IS NOT COMPLETE):

US   2008032917 07 FEB 2008
DE 102006035202 31 JAN 2008
EP      1882693 30 JAN 2008
JP   2008024674 07 FEB 2008
WO   2008021152 21 FEB 2008
GB      2439172 19 DEC 2007
FR      2904316 01 FEB 2008
RU      2316552 10 FEB 2008
CA      2593150 06 JAN 2008

Expanded G-group definition display now available.

Effective December 15th the iteration and answer limits in MARPAT
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FILE HCAPLUS

FILE COVERS 1907 - 26 Mar 2008 VOL 148 ISS 13
FILE LAST UPDATED: 25 Mar 2008 (20080325/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate substance identification.

FILE WPIX
FILE LAST UPDATED: 24 MAR 2008 <20080324/UP>
MOST RECENT THOMSON SCIENTIFIC UPDATE: 200820 <200820/DW>
DERWENT WORLD PATENTS INDEX SUBSCRIBER FILE, COVERS 1963 TO DATE

>>> IPC Reform backfile reclassification has been loaded to the end of November 2007. No update date (UP) has been created for the reclassified documents, but they can be identified by 20060101/UPIC and 20061231/UPIC, 20070601/UPIC, 20071001/UPIC and 20071130/UPIC. <<<

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>>> XML document distribution format now available - See HELP XMLDOC <<<

>>> ECLA Codes and Current US National Classifications have been added - see NEWS and HELP CHANGE <<<

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>>> Updated PDF files in the following links:
http://www.stn-international.de/stndatabases/details/ico_0801.zip
http://www.stn-international.de/stndatabases/details/epc_0801.zip
Supplement of all changed ECLA items:
http://www.stn-international.de/stndatabases/details/ecla_0802s.zip <<

FILE STNGUIDE
FILE CONTAINS CURRENT INFORMATION.
LAST RELOADED: Mar 21, 2008 (20080321/UP).

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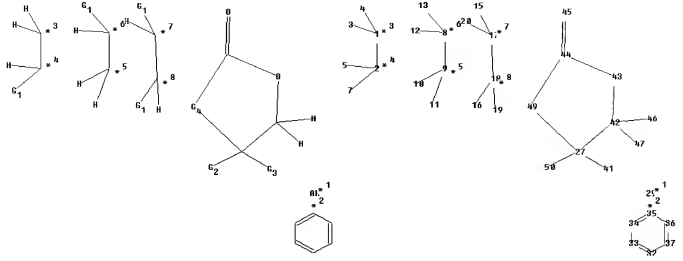

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ring nodes :
1 2 8 9 17 18 27 32 33 34 35 36 37 42 43 44 49
chain bonds :
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42-46 42-47 44-45
ring bonds :
1-2 8-9 17-18 27-49 27-42 32-33 32-37 33-34 34-35 35-36 36-37 42-43 43-44
44-49
exact/norm bonds :
1-3 1-4 2-5 2-7 8-12 8-13 9-10 9-11 15-17 16-18 17-20 18-19 27-41 27-50
42-46 42-47 44-45
exact bonds :
1-2 8-9 17-18 27-49 27-42 42-43 43-44 44-49
normalized bonds :
32-33 32-37 33-34 34-35 35-36 36-37

G1:CH3,Et

G2:CH3,H

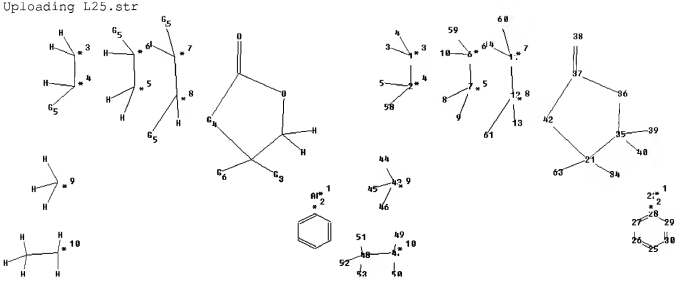
G3:[*1],[*2]

G4:[*3-*4],[*5-*6],[*7-*8]

Connectivity :
29:1 E exact RC ring/chain
Match level :
1:Atom 2:Atom 3:CLASS 4:CLASS 5:CLASS 7:CLASS 8:Atom 9:Atom 10:CLASS 11:CLASS
12:CLASS 13:CLASS 15:CLASS 16:CLASS 17:Atom 18:Atom 19:CLASS 20:CLASS
27:Atom 29:CLASS
32:Atom 33:Atom 34:Atom 35:Atom 36:Atom 37:Atom 41:CLASS 42:Atom 43:Atom
44:Atom 45:CLASS
46:CLASS 47:CLASS 49:Atom 50:CLASS

Element Count :
Node 29: Limited
C,C3

Uploading L25.str



chain nodes :
3 4 5 8 9 10 13 14 22 34 38 39 40 43 44 45 46 47 48 49 50 51 52 53 58 59 60 61 63
ring nodes :
1 2 6 7 11 12 21 25 26 27 28 29 30 35 36 37 42
chain bonds :
1-3 1-4 2-5 2-58 6-10 6-59 7-8 7-9 11-14 11-60 12-13 12-61 21-34 21-63 35-39 35-40 37-38 43-44 43-45 43-46 47-48 47-49 47-50 48-51 48-52 48-53
ring bonds :
1-2 6-7 11-12 21-42 21-35 25-26 25-30 26-27 27-28 28-29 29-30 35-36 36-37 37-42
exact/norm bonds :
1-3 1-4 2-5 2-58 6-10 6-59 7-8 7-9 11-14 11-60 12-13 12-61 21-34 21-63 35-39 35-40 37-38 43-44 43-45 43-46 47-48 47-49 47-50 48-51 48-52 48-53
exact bonds :
1-2 6-7 11-12 21-42 21-35 35-36 36-37 37-42
normalized bonds :
25-26 25-30 26-27 27-28 28-29 29-30

G3:[*1],[*2]

G4:[*3-*4],[*5-*6],[*7-*8]

G5:[*9],[*10]

G6:H,[*9]

Connectivity :
22:1 E exact RC ring/chain

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Match level :
1:Atom  2:Atom  3:CLASS  4:CLASS  5:CLASS  6:Atom  7:Atom  8:CLASS  9:CLASS
10:CLASS
11:Atom  12:Atom  13:CLASS  14:CLASS  21:Atom  22:Atom  25:Atom  26:Atom  27:Atom
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Element Count :
Node 22: Limited
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